

A STRUCTURAL STUDY OF A MIXED-VALENCE
COMPLEX OF COBALT AND DIACETYL-
OXIME-ANIL

A THESIS

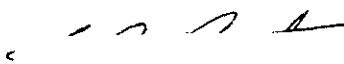
Presented to
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By
Thomas Edward Shaw, III

In Partial Fulfillment
of the Requirements for the Degree
Master of Science in Chemistry

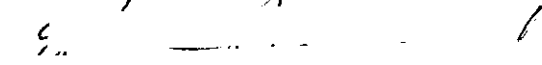
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A STRUCTURAL STUDY OF A MIXED-VALENCE
COMPLEX OF COBALT AND DIACETYL-
OXIME-ANIL


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J. A. Bertrand, Chairman



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Date approved by Chairman Aug 16, 1978

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SUMMARY

Bis[tris(2-phenylimino-3-oximo-butanato)cobalt(III)] cobalt(II) perchlorate was prepared and the structure determined via single crystal x-ray methods. The structure contains trinuclear cations and discrete perchlorate anions. The trinuclear cation consists of a central cobalt(II) ion located between two octahedrally coordinated tris(2-phenylimino-3-oximo-butanato)cobalt(III) groups. Each ligand is coordinated to cobalt(III) through the imine and oxime nitrogens with the six oxime oxygens of two such complexes octahedrally coordinating the central cobalt(II).

The temperature-independent magnetic moment from a previously published study is consistent with the presence of a high-spin, octahedrally coordinated cobalt(II) and two diamagnetic cobalt(III) ions.

CHAPTER I

INTRODUCTION

Although it is possible, on the basis of current understanding of the electronic states associated with d^n configurations, to predict the magnetic moment of most transition metal complexes, there are a number of complexes reported with anomalous magnetic moments. In recent years these compounds have received considerable attention and, on the basis of structure determinations and other studies, it has been possible to explain the "anomalous" behavior of many of these compounds. From these studies, there appear to be four distinct categories of complexes with "anomalous" moments. First, there are polynuclear complexes which contain metal-metal bonds. Examples include $\text{Re}_2\text{Cl}_8^{2-}$, $\text{Mn}_2(\text{CO})_{10}$, $\text{Co}_2(\text{CN})_{10}^{6-}$, $\text{Cu}_2(\text{O}_2\text{CCH}_3)_4(\text{H}_2\text{O})_2$, and $\text{Cr}_2(\text{O}_2\text{CCH}_3)_4(\text{H}_2\text{O})_2$.¹ Complexes of this type exhibit subnormal magnetic moments compared with values expected for isolated metal ions due to pairing of spins in metal-metal interactions. In the case of strong interactions, such complexes are diamagnetic. Second, there are polynuclear complexes which exhibit exchange interactions through bridging groups. Spin coupling can occur through a variety of bridging groups, but the most extensively studied complexes are oxygen-bridged

copper(II) complexes.² Third, there are cases in which the complex is incorrectly formulated as a single valence state. On the basis of mixed-valence, their "anomalous" magnetic properties can be explained. Complexes of the formula $[M(II)(H_2O)_6][M(III)(SALGLY)_2] \cdot 2H_2O$ (where $M = Co, Mn, Fe$)³⁻⁶ are representative examples (All abbreviations of ligands are listed in Tables 1 and 2). Finally, there are complexes which exhibit spin-state equilibria. In these complexes, high-spin and low-spin states have similar energies resulting in a thermal population of different spin states. Complexes of iron(III) containing dithiocarbamate ligands are the earliest examples and have been extensively studied in recent years.^{7,8}

Uhlig and Dinjus reported compounds of the formula $[Co(Dma)(Dma-H)B]ClO_4$ (where $B = C_5H_5N$ or $C_6H_5NH_2$).⁹ The magnetic moments reported for these compounds, ranging from 3.18 to 3.62 B.M., are considerably below the range expected for cobalt(II).

As an explanation for the unusual magnetic moments, Uhlig and Dinjus proposed that these complexes are dimeric in the solid state with a cobalt-cobalt bond. Cobalt(II) dimers with cobalt-cobalt bonds have been reported. $Co_2(CN)_{10}^{6-}$ and $Co_2(CNCH_3)_{10}^{4+}$ are examples.¹

The possibility of a mixed-valence compound of cobalt (II) and cobalt(III) was not considered, presumably because the preparations were carried out under an inert atmosphere.

Table 1. Abbreviations Used for Ligands

Deta	the dianion of 2,2'-dihydroxydiethylamine
Eta	the anion of 2-aminoethanol
Dma	the anion of diacetylmonoxime anil
SALGY	the dianion of the imine of salicylaldehyde and glycine

Table 2. Abbreviations Used for Ligands²

$\begin{array}{c} \text{CH}_3 \quad \text{CH}_3 \\ \diagdown \quad \diagup \\ \text{C} - \text{C} \\ \diagup \quad \diagdown \\ \text{O} - \text{N} = \quad \text{N} - (\text{CH}_2)_n - \text{X} \end{array}$					
LnX					
n will always be an integer					
<u>n</u>	<u>X</u>	<u>Symbol</u>	<u>n</u>	<u>X</u>	<u>Symbol</u>
n=2,3	OH	Lna ₂	0	$\text{NH}-\text{C} \begin{array}{l} \nearrow \text{O} \\ \searrow \text{NH}_2 \end{array}$	L0sc
n=2,3	NH ₂	Lnam			
2	α-pyridine	L2pyr			
2	(C ₂ H ₅) ₂ N	L2dea	0	$\text{NH}-\text{C} \begin{array}{l} \nearrow \text{S} \\ \searrow \text{SCH}_3 \end{array}$	L0dts
1	CH ₃	Let			
			3	$\begin{array}{c} \text{N} \quad \text{N-OH} \\ \diagdown \quad \diagup \\ \text{C} - \text{C} \\ \diagup \quad \diagdown \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$	L3LH

However, similar magnetic moments have been reported for compounds formulated as cobalt(II) when both cobalt(II) and cobalt(III) were present.

Structural and magnetic studies of mixed-valence cobalt compounds show that they fall into two categories. First, there are those which show temperature-dependent magnetic moments due to coupling between paramagnetic centers. And second, there are those which show temperature-independent magnetic moments due to the presence of a single paramagnetic center.

An example falling into the first category was reported by J. A. Bertrand and T. C. Hightower.¹⁰ Di- μ -acetato-tetrakis- $[\mu_3$ -methoxo-2,4-pentanedionatocobalt(II,III)] (abbreviated as Co-cubane, Figure 1) shows magnetic coupling (4.98 B.M. at room temperature and 4.62 B.M. at liquid N₂ temperature). Also, $[\text{Co(II)Co(III)(Deta)}_2(\text{Deta H}_2)]_2(\text{ClO}_4)_2$ (abbreviated as CoDeta) was reported by E. Fujita¹¹ with a structure similar to that of titanium alkoxides. It shows a temperature-dependent magnetic moment (5.19 B.M. at room temperature and 5.07 B.M. at 93°K) and thus, coupling between cobalt(II) ions. Both compounds contain a Co₂O₂ four membered ring (planar for CoDeta and bent for Co-cubane) permitting coupling between cobalt(II) ions, and additional bridging by the acetate ion in Co-cubane provides another possible coupling pathway.

An example falling into the second category, bis[tris

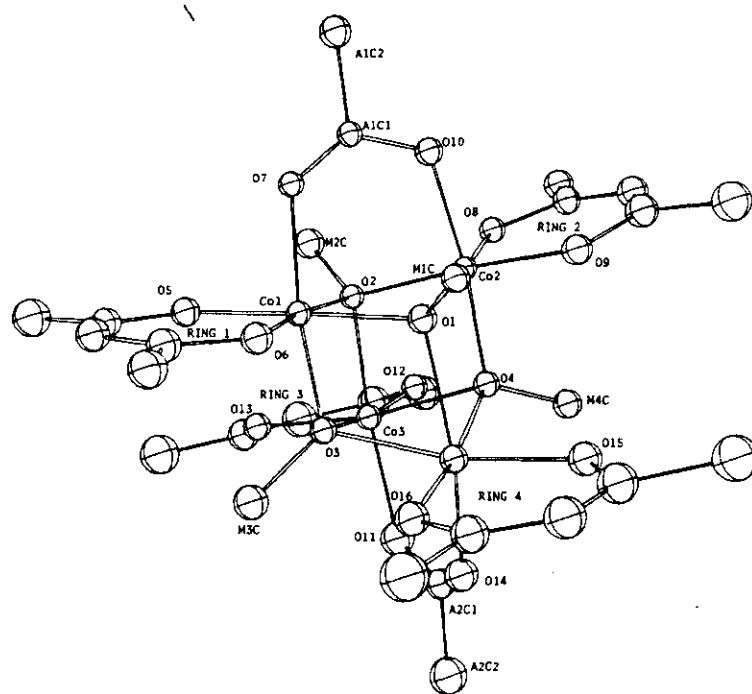


Figure 1. A Perspective Drawing of Co-Cubane

(2-aminoethoxido)cobalt(III)]cobalt(II), was reported by J. A. Bertrand, J. A. Kelley, and E. G. Vassian.¹² V. V. Vdovenko and A. N. Gerasenkova reported a series of trinuclear complexes with the formula $[\text{Co}_3(\text{Eta})_6]\text{X}_2 \cdot n\text{H}_2\text{O}$.^{13,14} One cobalt(II) and two cobalt(III) ions per formula unit were indicated by potentiometric analyses for cobalt(II) and for total cobalt, and a structure with face-sharing octahedra was proposed. The structural study of the trinuclear cobalt complex above confirmed both the face-sharing arrangement and the octahedral coordination of the terminal cobalt(III) ions (Figure 2). However, the six alkoxide oxygens coordinated to the central cobalt(II) in an almost perfect trigonal prismatic arrangement. The magnetic moment (4.05 B.M.) was consistent with three unpaired electrons and was temperature-independent.

Another polynuclear cobalt complex, $\text{NaCo}_6[(\text{DetaH}_2)_6 - 7\text{H}](\text{OH})_4(\text{CO}_3)_3 \cdot 12\text{H}_2\text{O}$, was prepared by A. Yao¹⁵ and a structural study was attempted. The ratio of cobalt(II) to cobalt(III) was 2:1 and a portion of the structure revealed an arrangement of cobalt atoms similar to the tetrameric unit present in titanium alkoxides (Figure 3).¹⁶⁻¹⁹ Two cobalt atoms were not located due to twinning, disordered atoms, and/or poor data.

The possibility of exchange coupling in the previously mentioned $[\text{Co}(\text{Dma})(\text{Dma-H})\text{B}]\text{ClO}_4$ compounds was not considered by Uhlig and Dinjus. However, the oxime groups of

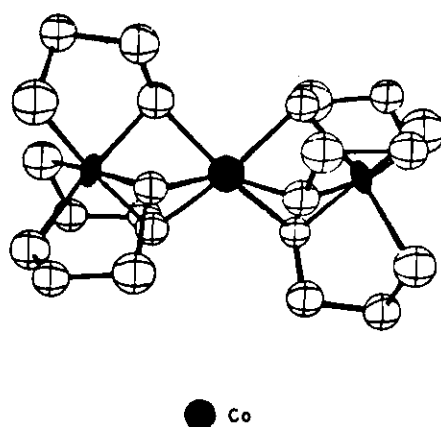


Figure 2. Structure of the Trinuclear Cobalt(II)-
Cobalt(III) Complex of 2-Aminoethanol

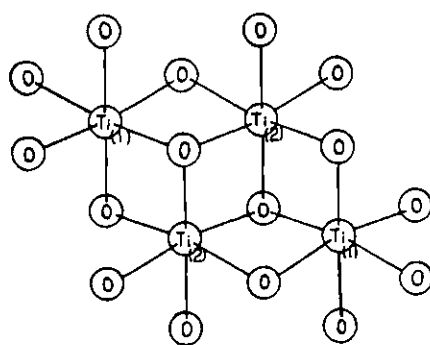


Figure 3. Structure of Titanium Alkoxides

similar ligands have formed bridges between metal ions and some of the resulting compounds exhibit spin coupling. For example, the structure of bis(dimethylglyoximate)copper(II), $\text{Cu}(\text{dmgH})_2$, was reported by A. Vaciago and L. Zamibonelli,²⁰ and that of bis(4,4,9,9-tetramethyl-5,8-diazadodecane-2,11-dione-2oxime- μ -11-oximate)dicopper(II)bromide, $\text{Cu}(4499)\text{Br}$, by J. W. Fraser, G. R. Hedwig, H. K. J. Powell, and W. T. Robinson.²¹ A dimeric nickel complex, bis[N-(6-amino-4-aza-3,3,6-trimethyl-2-heptylidenyl)hydroxanato]pentaquo dinickel(II)chloride or $\text{Ni}(\text{NAH})\text{Cl} \cdot 2.5\text{H}_2\text{O}$, was reported by E. O. Schlemper and R. K. Murmann,²² and a complex with a reduced magnetic moment, μ_3 -hydroxo-tri- μ -(pyridine-2-carbaldehyde oximate)- μ_3 -sulphato-tricopper(II)-16.3 water or $[\text{Cu}_3(\text{pyal})_2\text{OH}]\text{SO}_4 \cdot 16.3\text{H}_2\text{O}$, was reported by R. Beckett and B. F. Hoskins.²³

Several interesting oxime-bridged copper complexes have been reported using imine ligands derived from 2,3-butanedione monoxime. The synthesis of $\text{Cu}(\text{L2py})\text{ClO}_4$ was reported by V. E. Uhlig and D. Schneider in 1964.²⁴ A. V. Ablov and N. I. Belichuk reported $\text{Cu}(\text{L2al})\text{ClO}_4 \cdot \text{H}_2\text{O}$.²⁵ And in 1974, the synthesis of $[\text{Cu}(\text{Let})_3\text{O}]\text{ClO}_4$ and $[\text{Cu}(\text{L2dea})(\text{ClO}_4)]_2 \cdot \text{H}_2\text{O}$ was reported by J. G. Mohanty, S. Baral, R. P. Singh, and A. Chakravorty.²⁶ Also, $\text{Cu}(\text{LOsc})(\text{ClO}_4)$ was reported by A. V. Ablov and N. I. Belichuk.²⁷

More recently, several new complexes involving imine ligands derived from 2,3-butanedione monoxime have been

synthesized and studied. $\text{Cu}(\text{L3al})(\text{ClO}_4) \cdot \text{H}_2\text{O}$, $\text{Cu}(\text{L3am})(\text{ClO}_4)$, and $\text{Cu}(\text{LOdts})\text{Br}$ have been synthesized.² In addition, structures have been reported for $\text{Cu}(\text{L2am})(\text{ClO}_4)$,²⁸ $\text{Cu}(\text{L3LH})(\text{ClO}_4) \cdot \frac{1}{2}\text{CH}_3\text{OH}$,²⁹ and the previously reported $\text{Cu}(\text{L2al})(\text{ClO}_4) \cdot \text{H}_2\text{O}$ ³⁰ and $\text{Cu}(\text{L2py})(\text{ClO}_4) \cdot \text{CH}_3\text{CN}$.²⁸

Thus, the magnetic properties of the compounds reported by Uhlig and Dinjus could result from metal-metal bonds, exchange coupling, or mixed-valence. In order to determine the actual cause of the unusual magnetic moments, a structural study was undertaken.

CHAPTER II

EXPERIMENTAL

Preparation of $[\text{Co}_3(\text{Dma})_6](\text{ClO}_4)_2$

The method of Uhlig and Dinjus⁹ for the synthesis of $[\text{Co}(\text{Dma})(\text{Dma-H})(\text{C}_5\text{H}_5\text{N})]\text{ClO}_4$ or $[\text{Co}(\text{Dma})(\text{Dma-H})(\text{C}_6\text{H}_5\text{NH}_2)]\text{ClO}_4$ yielded a red brown powder. Dark red prismatic crystals were obtained by recrystallization from absolute ethanol. Anal. Calc'd for $\text{Co}_3(\text{C}_{60}\text{H}_{66}\text{N}_{12}\text{O}_6)(\text{ClO}_4)_2$: C, 50.50; H, 4.67; N, 11.78; Cl, 4.97. Found: C, 47.35; H, 4.92; N, 11.05; Cl, 5.45. Elemental analyses were performed by Atlantic Micro-lab, Inc. in Atlanta, Georgia.

Crystallographic StudiesCrystallographic Data Collection

Since crystals of the compound lost weight and cracked upon exposure to air, the data were collected on crystals sealed in epoxy. The observation of a significant drop in the intensities of three standard reflections required that data be collected on two crystals. The data set from one crystal was scaled to that of the other by a comparison of standard reflections.

A red (epoxy coated) crystal with approximate dimensions .30 x .40 x .70 mm. (.50 x .50 x 1.15 for the second crystal) was mounted on a glass fiber using epoxy cement

such that the longest crystal dimension was approximately parallel to the fiber axis.

Unit cell parameters and the orientation matrix were determined on a Syntex P2₁ four circle diffractometer equipped with a graphite monochromator (Bragg 2 θ angle = 12.2°) using MoK α radiation at a takeoff angle of 6.75°. Fifteen reflections whose 2 θ values ranged from 6.03° to 19.24° (5.75° to 22.60° for the second crystal) were machine-centered and used in least-squares refinement of the lattice parameters and orientation matrix. Unit cell parameters obtained were $a = 17.81(2)\text{\AA}$,³¹ $b = 15.056(4)\text{\AA}$, $c = 28.37(2)\text{\AA}$, $\beta = 92.06(6)^\circ$, and $V = 7604(9)\text{\AA}^3$ [$a = 17.81(1)\text{\AA}$, $b = 15.06(4)\text{\AA}$, $c = 28.37(3)\text{\AA}$, $\beta = 92.05(7)^\circ$, and $V = 7605(10)\text{\AA}^3$ for the second crystal]. The calculated density of 1.25 g cm⁻³ for four formula units per unit cell does not agree with the experimental density of 1.39 g cm⁻³ measured by the flotation method using a mixture of ethanol and carbon tetrachloride. Omega scans of several low 2 θ angle reflections gave peak widths at half-height of less than .29°, indicating a satisfactory mosaic spread for the crystal (also .29° for the second crystal).

Intensity data for zero and upper levels were collected at a rapid scan rate and the intensities examined carefully for systematic absences. The absence of $h0\ell$ reflections with $\ell = 2n + 1$ and $0k0$ reflections with $k = 2n + 1$ is consistent only with space group P2₁/c (No. 14).³²

Intensity data were collected using θ - 2θ scans with x-ray source and monochromator settings identical to those used for determination of the unit cell parameters. A variable scan rate of from 4.88° to 29.30° min (5.86° to 29.30° min for the second crystal) was used and a scan width of 2.00° was sufficient to collect all of the peak intensity. Stationary background counts were measured at the beginning (bgd1) and at the end (bgd2) of each scan with a total background to scan time ratio, TR, of 1.0. No significant fluctuations were observed in the intensities of three standard reflections (4,0,0; 0,4,0; 0,0,4) monitored every 97 reflections (except when the first crystal failed and the remainder of the data were collected using a second crystal). Intensities were calculated from the total scan count (CT) and background counts by the relationship:

$$I = CT - (TR)(bgd1 + bgd2).$$

The intensities were assigned standard deviations according to the formula

$$\sigma(I) = [CT + (TR)^2(bgd1 + bgd2)]^{\frac{1}{2}}$$

from a total of 14391 reflections collected in a complete quadrant ($-h \rightarrow h$, $0 \rightarrow k$, $0 \rightarrow l$) of data out to $2\theta = 50.0^\circ$; 4079 were accepted as statistically above background on the basis that I was greater than $3\sigma(I)$. Lorentz and polarization corrections were made in the usual way.

Solution and Refinement of the Structure

Computations were performed using standard programs;³³

all computations were carried out on the CDC Cyber 74 System. For structure factor calculations the scattering factors were taken from Cromer and Waber's tabulation³⁴ for all atoms except hydrogen; Stewart's hydrogen atom scattering factors³⁵ were used. The scattering factors for Co, Cl were corrected for the real and imaginary anomalous dispersion components, using the dispersion factors given by Cromer.³⁶ The agreement factors are defined in the usual way as

$$R = (\sum ||F_O| - |F_C||) / (\sum |F_O|)$$

and

$$R_w = [\sum_w (|F_O| - |F_C|)^2 / \sum_w (|F_O|)^2]^{1/2}$$

In all least squares refinements, the quantity minimized was $w(|F_O| - |F_C|)^2$. A weighting scheme based on counting statistics ($w = 4I/\sigma^2(I)^2$) was employed for calculating R_w and in least-squares refinement.

Coordinates for two cobalt atoms were obtained from a three-dimensional Patterson synthesis. Two cycles of full-matrix least-squares refinement of the coordinates and isotropic temperature factors for these atoms resulted in R of 0.48 and R_w of 0.477. The remaining cobalt, oxygen, nitrogen, carbon, and chlorine atoms were located by means of subsequent difference Fourier calculation and least-squares refinement. A refinement using the weighting scheme and using anisotropic temperature factors for cobalt, chlorine, oxygen, and nitrogen atoms was used. The six phenyl rings were refined as rigid groups varying x, y, z of the center of the ring and three

orientation angles. The temperature factors for carbon were varied individually. Similarly, the two perchlorate groups were refined as rigid groups varying the oxygen temperature factors independently and the position of the group as a whole. One of the perchlorate groups was refined as two half groups due to disorder. The positions for hydrogen were calculated and the phenyl hydrogens refined as part of the groups. Neither the hydrogen coordinates nor the thermal parameters (fixed at 5.0) were varied. The refinement converged to final values of $R = 0.087$ and $R_w = 0.097$. In the final cycle of refinement, the maximum parameter shift was 0.009σ (Z coordinate of Co3). The major feature on a final difference Fourier map was a peak of $1.35 \text{ e}\text{\AA}^{-3}$. This position was not located near any atoms in the structure and would not refine. The final structural parameters are listed in Table 3 and the final observed and calculated structure factors are listed in Table 4.

Table 3. Positional and Thermal Parameters for $[\text{Co}_3(\text{Dma})_6](\text{ClO}_4)_2$

ATOM	x	y	z	B11	B22	B33	B12	B13	B23
CO1	.1463(19)	.114(1)	.2704(17)	2.63(8)	3.0(1)	2.49(9)	-.16(9)	.01(7)	.13(9)
CO2	-.1614(19)	.1057(12)	.0992(17)	2.49(8)	3.6(1)	2.54(9)	-.25(8)	-.10(7)	.05(9)
CO3	.1171(1)	.1067(2)	.1519(17)	2.65(8)	3.6(1)	2.92(9)	-.05(9)	-.19(6)	-.1(1)
CL1	-.3721(13)	.1630(4)	.3142(2)	6.7(13)	6.2(13)	6.1(13)	.1(2)	.0(2)	-.7(3)
CL2	.1485(14)	.1498(5)	.4957(2)	10.7(14)	9.4(14)	6.2(13)	2.0(13)	2.0(13)	-.3(3)
L1O1	.1538(15)	-.0778(17)	.1402(4)	3.4(15)	4.2(16)	4.1(16)	.1(4)	-1.3(4)	.3(5)
L2O1	-.1764(15)	.1749(7)	.1773(4)	2.6(4)	4.9(16)	3.6(15)	-.4(4)	.0(4)	-1.2(5)
L3O1	-.0118(15)	.1483(7)	.0813(4)	2.6(4)	4.7(16)	4.0(16)	.3(4)	.3(4)	.5(5)
L4O1	.0508(15)	.2214(7)	.1561(4)	2.9(4)	3.8(15)	3.5(15)	.5(4)	.1(4)	.7(4)
L5O1	.3462(15)	.0771(7)	.2217(3)	3.3(4)	4.4(16)	2.6(15)	-.5(4)	-.5(3)	.3(4)
L6O1	.1185(15)	.0295(16)	.1294(3)	2.8(4)	3.2(15)	3.1(15)	-.3(4)	-.9(3)	-.3(4)
L1N1	-.1773(16)	.0590(9)	.3335(4)	3.0(15)	4.3(17)	2.6(16)	.4(15)	.3(4)	-.4(5)
L1N6	.1957(16)	.0358(8)	.1033(4)	2.7(15)	3.1(16)	3.5(16)	-.2(15)	.0(15)	-.1(5)
L2N1	-.2439(16)	.0401(8)	.1277(4)	3.0(15)	3.9(17)	2.3(16)	-.1(15)	-.2(4)	.2(5)
L2N6	-.1384(15)	.1329(8)	.1637(4)	2.1(15)	4.1(17)	2.9(15)	.1(4)	.2(4)	-.4(5)
L3N1	-.2162(16)	.2184(8)	.0851(4)	2.4(15)	4.0(17)	3.2(16)	-.2(15)	-.2(4)	.3(5)
L3N6	-.1604(16)	.1793(9)	.0885(4)	2.7(15)	4.6(17)	2.6(16)	.1(15)	-.0(4)	-.3(5)
L4N1	.2634(16)	.1224(8)	.1996(4)	3.2(15)	3.5(17)	3.1(16)	-.6(15)	.2(4)	.2(5)
L4N6	.1559(16)	.1951(10)	.1958(4)	2.3(15)	3.0(16)	3.3(16)	.5(4)	.0(4)	.5(5)
L5N1	.2272(16)	.2104(8)	.2445(4)	2.8(15)	4.0(17)	2.9(16)	-.3(15)	.1(4)	-.1(5)
L5N6	.1373(15)	.1210(8)	.2347(4)	2.6(15)	3.1(16)	2.6(15)	.0(15)	-.0(4)	.2(5)
L6N1	.2377(16)	.0158(8)	.2398(4)	3.1(15)	3.6(16)	2.1(16)	.3(15)	-.7(4)	.2(5)
L6N6	.1559(16)	.0176(8)	.1656(4)	2.6(15)	2.7(16)	3.0(16)	.5(4)	.1(4)	-.3(5)

ATOM	x	y	z	B
L1C2	-.1392(18)	-.011(1)	.0260(6)	3.8(13)
L1C3	-.1411(1)	-.263(1)	-.0251(7)	5.7(14)
L1C4	-.0885(18)	-.043(1)	.0649(16)	3.5(13)
L1C5	-.0311(1)	-.114(2)	.0622(17)	6.2(14)
L2C2	-.2424(17)	.047(1)	.1736(15)	3.2(13)
L2C3	-.3033(19)	.003(1)	.2444(16)	4.2(13)
L2C4	-.1814(17)	.698(1)	.1946(15)	3.3(13)
L2C5	-.1665(19)	.109(1)	.2476(16)	5.2(14)
L3C2	-.1748(18)	.282(1)	.0767(16)	4.1(13)
L3C3	-.199(1)	.376(1)	.0678(17)	6.2(14)
L3C4	-.0965(18)	.259(1)	.0702(16)	3.4(13)
L3C5	-.436(1)	.327(1)	.0553(17)	5.6(14)
L4C2	.2714(18)	.180(1)	.1242(16)	3.6(13)
L4C3	.3288(19)	.196(1)	.0862(17)	5.4(14)
L4C4	.2633(18)	.222(1)	.1220(16)	3.6(13)
L4C5	.1726(19)	.286(1)	.0837(17)	5.2(14)
L5C2	.1779(18)	.225(1)	.2753(16)	3.9(13)
L5C3	.1854(19)	.295(1)	.3145(17)	5.3(14)
L5C4	.1381(18)	.175(1)	.2706(16)	3.6(13)
L5C5	.1389(19)	.186(1)	.3004(17)	4.9(14)
L6C2	.2177(18)	-.060(1)	.2238(16)	3.6(13)
L6C3	.240(1)	-.149(1)	.2469(17)	5.0(14)
L6C4	.1703(18)	-.063(1)	.1817(16)	3.3(13)
L6C5	.135(1)	-.144(1)	.1587(17)	5.8(14)

$$[\text{Co}_3(\text{Dma})_6](\text{ClO}_4)_2$$
[illegible]

Table 4. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	
6	9	43	46	2	8	50	54	7	16	71	66	2	13	101	102	7	9	30	28	1	11	121	119	5	17	32	30	13	5	51	46	13	5	51	46	
6	17	86	90	2	10	73	66	7	20	35	32	2	15	80	79	7	9	32	34	1	12	40	44	5	25	46	47	13	6	54	56	13	6	54	56	
6	18	36	41	2	12	69	69	8	2	46	44	2	17	48	47	7	10	52	51	1	13	47	50	5	27	51	50	13	7	55	58	13	7	55	58	
6	19	77	74	2	13	66	69	8	7	48	56	2	19	35	33	7	12	94	96	1	15	34	34	6	1	52	54	13	10	38	37	13	10	38	37	
6	23	39	41	2	15	51	53	8	8	45	52	2	29	36	35	7	11	40	45	1	20	34	38	6	3	45	47	13	11	55	55	13	11	55	55	
7	2	50	45	2	16	36	40	8	10	34	37	3	2	28	18	7	14	38	44	2	1	29	32	6	4	33	36	14	4	36	41	14	4	36	41	
7	5	35	32	2	17	93	89	8	13	36	40	3	3	43	44	7	16	38	36	2	2	52	56	6	5	46	41	14	8	70	70	14	8	70	70	
7	6	35	36	2	19	49	57	9	3	44	41	3	4	85	79	8	4	31	31	2	3	47	55	6	6	61	68	14	12	48	37	14	12	48	37	
7	7	32	31	3	1	93	94	9	5	31	26	3	5	70	68	8	9	46	49	2	4	45	45	6	7	58	66	15	11	39	37	15	11	39	37	
7	16	44	47	3	2	53	48	9	7	49	50	3	7	43	34	8	12	53	55	2	5	76	69	6	8	64	69									
7	20	63	62	3	3	44	47	9	9	36	42	3	8	36	35	8	13	47	55	2	7	118	110	6	9	114	121									
7	22	54	54	3	5	36	38	9	15	36	32	3	10	82	84	8	14	43	45	2	8	53	57	6	11	32	31									
8	1	30	38	3	6	61	60	10	1	34	36	3	11	35	47	9	1	30	27	2	9	150	138	6	12	42	42									
8	6	31	33	3	7	33	27	10	7	39	39	3	12	81	79	9	6	35	31	2	10	36	28	6	13	29	19									
8	7	43	40	3	8	27	24	10	8	48	46	3	16	64	63	9	9	54	52	2	11	35	37	6	17	56	59									
8	10	39	35	3	9	78	68	10	11	48	49	3	17	43	38	9	11	72	78	2	12	33	29	6	18	32	35									
8	13	36	35	3	14	55	56	11	6	51	52	3	25	37	29	9	13	57	52	2	13	69	73	7	2	81	76									
9	1	56	53	3	16	83	85	11	9	35	34	3	30	50	45	10	1	83	89	2	19	58	60	7	4	43	35									
9	3	35	40	3	19	31	32	11	10	39	43	4	2	83	72	10	3	62	58	2	27	39	38	7	6	33	35									
9	8	35	41	3	23	53	49	11	12	36	30	4	5	80	81	10	5	41	40	2	29	57	58	7	8	53	50									
9	21	55	53	4	1	46	51	11	15	36	36	4	8	92	98	10	7	34	36	3	1	27	39	7	10	94	92									
10	11	37	41	4	4	42	45	11	16	57	56	4	9	55	61	10	8	33	42	3	2	74	65	7	12	60	60									
11	2	35	40	4	7	33	33	12	13	61	62	4	10	27	35	10	12	55	51	3	3	56	53	7	13	48	47									
11	12	34	32	4	11	28	22	13	5	45	42	4	11	27	28	10	13	40	34	3	4	42	45	7	15	73	74									
11	20	48	42	4	12	32	31	13	15	48	41	4	12	47	45	10	14	35	34	3	5	104	95	7	16	53	51									
12	3	42	39	4	13	33	37	13	16	41	40	4	13	56	66	11	9	34	24	3	6	194	194	7	26	51	52									
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13	1	68	66	4	18	77	78					4	20	31	22	12	2	55	53	3	10	104	115	8	8	54	50									
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				5	1	40	44					5	1	126	135	12	9	71	69	3	12	74	68	8	10	71	69									
				5	2	71	69					5	2	87	84	12	13	69	69	3	26	38	39	8	16	39	38									
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				5	14	35	35					5	8	26	24	14	14	56	47	4	5	131	115	9	11	43	49									
				5	15	118	118					5	9	43	45					4	6	51	43	9	13	37	37									
				5	17	80	83					5	10	34	38					4	8	166	159	9	14	43	42									
				5	19	34	30					5	11	103	104					4	9	41	48	9	25	36	32									
				6	1	50	50					5	15	66	66					4	10	52	55	10	7	75	78									
				6	2	28	19					5	18	32	36					4	14	58	54	18	8	106	105									
				6	3	31	39					5	21	53	45					4	18	41	46	10	9	85	81									
				6	6	43	47					6	3	37	44					4	28	55	54	10	10	56	55									
				6	7	43	45					6	4	40	41					5	2	47	50	10	11	48	54									
				6	10	63	65					6	5	53	45					5	3	78	70	11	6	97	102									
				6	13	34	32					6	6	87	88					5	4	83	74	11	8	39	41									
				6	14	40	42					6	9	58	56					5	5	101	98	11	10	59	59									
				6	17	53	49					6	12	82	82					5	6	91	89	11	12	70	65									
				6	18	53	52					6	13	108	104					5	7	109	110	12	1	37	38									
				6	19	35	37					6	14	41	45					5	8	29	31	12	7	69	77									
				7	2	32	36					6	16	42	42					1	5	180	178	12	8	69	61									
				7	6	48	52					7	2	44	38					5	13	59	62	12	9	116	115									
				7	7	31	42					7	3	32	33					1	7	200	205	12	10	51	49									
				7	10	32	38					7	4	30	38					5	13	39	32	12	13	47	48									
				7	12	33	36					7	7	50	54					1	1	74	82	13	4	36	35									

H= -7

0	2	82	92
0	4	266	261
0	8	153	137
10	10	152	151
12	12	62	68
16	16	56	55
18	18	36	33
20	20	92	91
22	22	32	40
24	24	34	30
2	1	98	82
2	2	112	181
5	5	113	112
6	6	119	120
7	7	194	203
8	8	93	64
9	9	76	74
10	10	32	42
11	11	34	35
12	12	37	40
15	15	38	31
22	22	32	38
23	23	50	44
26	26	67	61
27	27	37	38
2	2	110	180
3	3	217	220
4	4	58	55
5	5	114	101
6	6	58	61
7	7	64	68
9	9	152	152
11	11	48	42
12	12	25	33
13	13	35	35
14	14	36	38
15	15	34	29
16	16	39	35
17	17	61	64
19	19	45	44
21	21	49	55
23	23	56	52
1	1	33	29
2	2	92	110

Table 4. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	
3	3	103	102	7	11	31	40	0	4	143	174	3	16	62	62	8	7	50	42	1	16	83	89	5	4	29	25	12	9	32	38					
3	4	59	53	7	13	33	33	0	6	89	103	3	17	29	28	8	11	40	44	1	17	111	118	5	5	102	87	12	15	38	48					
3	5	51	63	7	16	59	63	0	8	208	202	3	18	64	66	8	12	61	62	1	21	63	61	5	6	48	50	12	19	55	54					
3	6	204	195	7	19	37	36	0	10	104	101	3	20	40	44	8	14	48	46	1	22	45	37	5	7	58	61	13	1	47	46					
3	7	126	134	7	22	51	53	0	12	27	31	3	21	41	43	8	21	47	45	2	1	62	14	5	8	73	79	13	3	41	49					
3	8	45	61	7	26	55	55	0	16	106	100	3	22	92	94	8	23	49	52	2	2	44	44	5	9	26	20	13	5	35	28					
3	11	36	22	8	3	28	36	0	18	115	102	3	23	74	73	9	1	153	147	2	4	27	24	5	12	48	46	13	17	61	57					
3	11	27	32	8	4	59	65	0	20	122	122	4	1	65	70	9	2	37	38	2	5	47	55	5	15	125	128									
3	13	26	28	8	5	92	87	0	22	42	35	4	2	96	105	9	3	85	88	2	6	61	68	5	17	134	138									
3	17	34	26	8	7	36	33	0	24	57	61	4	3	100	97	9	5	54	55	2	7	94	80	5	19	15	37									
3	19	38	28	8	8	40	35	1	1	181	145	4	4	244	242	9	7	51	51	2	8	157	139	5	21	60	59									
3	22	57	59	8	9	30	37	1	2	138	123	4	15	40	45	9	9	34	30	2	9	80	84	5	22	32	37									
3	26	58	51	8	12	64	67	1	3	171	157	4	17	41	38	9	10	47	45	2	10	41	31	6	2	67	76									
3	27	43	40	8	13	51	45	1	4	103	72	4	18	72	71	9	11	61	59	2	11	128	138	6	3	77	84									
4	1	67	73	8	14	77	78	1	5	94	89	4	19	61	64	9	21	57	49	2	12	112	106	6	4	86	102									
4	3	69	61	8	15	40	46	1	6	132	124	4	20	70	66	10	3	30	24	2	13	35	25	6	5	68	73									
4	4	231	233	8	23	41	42	1	7	23	27	4	21	48	48	10	4	66	72	2	14	45	38	6	6	30	29									
4	5	38	49	8	24	47	41	1	8	40	42	5	1	176	192	10	10	38	36	2	15	98	108	6	12	48	42									
4	7	55	57	8	25	39	46	1	9	62	61	5	3	72	77	10	24	37	31	2	17	64	66	6	14	60	55									
4	8	130	116	9	3	34	38	1	10	31	34	5	5	135	134	11	1	40	40	2	19	195	197	6	15	102	112									
4	10	40	45	9	5	56	57	1	11	112	122	5	7	204	97	11	2	113	112	3	1	163	155	6	17	36	40									
4	14	29	35	9	7	32	35	1	12	60	61	5	13	28	32	11	10	36	34	3	2	189	164	6	19	110	110									
4	28	42	38	9	10	39	33	1	13	38	34	5	15	51	55	12	22	42	41	3	3	47	40	6	27	36	33									
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5	1	168	149	9	27	38	36	1	18	81	82	5	21	50	54	12	10	33	30	3	6	123	110	7	13	71	69									
5	2	63	61	10	3	30	29	1	20	34	37	6	2	39	35	12	19	42	44	3	9	98	81	7	15	35	35									
5	3	145	144	10	4	62	64	1	21	84	87	6	1	32	39	13	1	41	29	3	10	34	39	7	16	146	144									
5	5	182	175	10	5	70	67	1	22	92	92	6	2	29	33	13	7	33	32	3	11	43	37	7	18	72	69									
5	6	86	89	10	7	36	35	1	23	77	70	6	3	109	109	13	21	49	45	3	13	75	67	7	20	49	53									
5	7	140	141	10	8	39	39	1	25	36	33	6	4	56	72	16	3	42	37	3	14	52	45	7	26	34	31									
5	8	43	46	10	11	61	68	2	1	56	50	6	5	77	74																					
5	14	51	54	10	13	75	74	2	3	198	209	6	6	79	86																					
5	15	44	44	10	15	39	39	2	5	75	70	6	8	34	36																					
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5	20	33	28	11	6	101	99	2	7	36	28	6	13	73	75																					
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6	1	71	69	11	11	48	44	2	10	37	35	6	17	48	48																					
6	3	105	99	12	3	40	41	2	16	31	39	6	18	63	66																					
6	4	109	119	12	4	33	35	2	17	40	44	6	19	89	91																					
6	5	73	72	12	5	88	82	2	18	51	54	6	20	36	36																					
6	7	52	55	12	6	33	30	2	19	152	157	6	23	37	33																					
6	8	64	69	12	9	64	65	2	21	48	45	7	2	166	165																					
6	9	40	40	12	10	34	29	2	21	37	47	7	6	84	84																					
6	13	32	35	12	12	35	34	2	23	64	62	7	10	26	31																					
6	14	66	74	13	2	34	32	3	1	50	37	7	11	29	30																					
6	15	60	56	13	5	54	48	3	2	233	230	7	12	95	96																					
6	23	57	55	13	6	37	40	3	3	36	41	7	13	64	64																					
6	24	59	49	13	7	58	64	3	4	34	29	7	18	32	30																					
6	28	37	37	14	4	60	58	3	5	130	144	7	20	36	39																					
7	2	69	72	14	8	55	51	3	6	53	58	7	22	67	72																					
7	3	32	30	15	6	40	38	3	7	27	26	8	1	60	63																					
7	6	143	143					3	9	100	102	8	2	32	29																					
7	7	45	43					3	10	24	33	8	3	76	77																					
7	8	29	36					3	12	31	36	8	4	65	61																					
7	14	52	46					3	15	45	48	8	5	50	40																					

M = -4

M = -5

Table 4. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
3	5	71	47	7	5	37	37	0	4	297	367	3	6	43	59	6	12	33	43	11	5	45	45	2	11	35	45	6	4	61	55
3	6	91	82	7	6	27	24	0	6	24	45	3	7	29	53	6	14	78	85	11	6	57	58	2	12	30	22	6	5	136	133
3	7	82	101	7	7	38	41	0	8	105	134	3	8	33	52	6	15	75	80	11	7	64	54	2	13	46	43	6	6	96	107
3	8	84	93	7	8	26	36	0	10	162	166	3	9	93	79	6	16	43	44	11	8	95	98	2	14	23	27	6	7	36	49
3	9	36	22	7	10	61	65	0	12	43	62	3	10	49	60	6	17	29	33	11	10	31	38	2	15	42	37	6	8	45	49
3	11	35	42	7	12	170	171	0	14	274	252	3	11	113	119	6	19	30	28	11	11	38	41	2	17	45	51	6	9	60	68
3	12	174	175	7	14	56	55	0	16	37	39	3	12	156	147	6	19	53	55	11	12	37	37	2	18	41	46	6	10	66	69
3	13	59	60	7	16	72	70	0	20	48	44	3	13	75	62	6	21	34	34	12	1	33	26	2	23	54	62	6	11	86	80
3	14	50	46	7	18	88	91	0	28	61	59	3	14	30	37	7	1	28	27	12	2	60	55	2	25	95	96	6	12	72	74
3	16	135	136	7	19	37	26	0	30	75	81	3	15	27	42	7	4	78	77	12	8	35	32	2	29	48	56	6	13	35	28
3	17	71	78	8	4	25	27	1	1	81	71	3	16	66	74	7	6	91	105	12	9	86	83	3	1	143	171	6	18	52	55
3	18	90	85	8	7	41	47	1	2	90	126	3	19	37	45	7	8	175	177	12	13	25	31	3	2	43	17	6	19	51	68
3	21	32	23	8	8	51	53	1	3	143	173	3	20	75	74	7	12	170	178	13	1	34	34	3	3	70	80	6	21	35	32
3	32	60	55	8	10	43	53	1	4	108	89	3	22	63	59	7	13	52	45	13	6	33	33	3	4	200	224	6	25	37	46
4	2	116	115	8	11	60	60	1	7	97	89	3	23	71	69	7	14	65	70	13	7	33	28	3	5	56	61	7	1	57	66
4	3	60	50	8	13	75	78	1	8	67	80	3	28	44	44	7	22	39	41	13	13	35	33	3	6	82	89	7	3	51	69
4	4	29	9	8	14	95	101	1	9	50	37	3	32	50	50	7	26	37	32	14	10	54	47	3	7	162	162	7	4	70	51
4	5	43	26	8	15	55	52	1	10	72	86	4	1	132	85	8	1	77	75	16	9	50	51	3	9	64	58	7	5	24	17
4	6	54	43	8	16	46	46	1	11	123	132	4	2	89	78	8	2	29	35	16	11	36	35	3	10	33	30	7	6	107	103
4	7	125	143	8	17	46	51	1	12	105	107	4	3	26	24	8	3	26	22	3	13	30	22	3	13	30	22	7	8	139	133
4	8	25	50	8	19	45	45	1	13	157	146	4	5	109	85	8	5	56	52					3	14	37	50	7	9	45	50
4	9	22	18	9	4	40	36	1	15	28	40	4	6	94	110	8	6	32	35					3	15	34	33	7	10	38	31
4	10	29	25	9	9	34	28	1	16	45	41	4	8	75	67	8	7	34	32	0	2	184	135	3	16	33	38	7	11	29	34
4	11	83	78	9	11	84	85	1	17	44	53	4	9	68	70	8	9	97	97	0	4	259	248	3	20	63	74	7	12	20	31
4	13	49	54	9	13	119	115	1	18	62	57	4	10	128	138	8	10	76	89	0	6	79	26	4	1	202	139	7	13	27	19
4	14	210	220	9	15	63	63	1	19	47	49	4	11	74	79	8	11	74	76	0	8	89	41	4	2	286	258	7	15	35	29
4	16	125	122	9	16	33	25	1	21	35	42	4	13	110	115	8	13	121	123	0	12	116	114	4	3	42	29	7	19	37	38
4	18	94	88	9	17	87	91	1	22	44	42	4	14	87	82	8	14	46	41	0	14	56	67	4	5	57	82	7	20	38	38
5	1	107	97	10	1	35	28	1	24	46	48	4	17	105	111	8	15	76	79	0	16	61	70	4	6	47	32	8	1	24	27
5	3	23	30	10	4	46	43	1	27	54	54	4	18	53	67	8	16	35	33	0	18	30	31	4	7	87	85	8	2	74	85
5	4	53	60	10	5	53	55	1	31	48	47	4	19	76	82	9	1	25	36	0	24	99	102	4	8	76	83	8	4	125	132
5	5	28	19	10	8	34	21	2	1	138	76	4	20	123	123	9	4	74	76	0	26	82	83	4	9	88	74	8	5	132	129
5	6	23	40	10	10	74	68	2	2	105	95	4	23	36	31	9	5	30	31	0	30	60	63	4	10	82	82	8	6	118	128
5	11	39	56	10	13	34	40	2	3	96	92	4	30	43	45	9	7	82	88	1	1	25	36	4	11	37	38	8	7	56	67
5	11	44	42	10	14	92	95	2	4	44	81	5	5	120	125	9	9	101	105	1	2	53	57	4	13	45	46	8	9	134	136
5	12	50	55	10	15	43	51	2	5	336	304	5	6	31	40	9	11	93	104	1	3	144	179	4	16	38	39	8	10	80	98
5	13	135	140	11	2	78	71	2	6	65	20	5	7	86	66	9	12	47	44	1	6	98	92	4	17	45	46	8	11	63	57
5	15	52	55	11	4	43	39	2	7	22	24	5	9	72	63	9	13	90	90	1	7	208	127	4	18	38	27	8	17	33	22
5	17	192	154	11	5	53	53	2	8	94	75	5	10	104	107	9	16	31	22	1	8	176	157	4	19	39	42	8	19	33	26
5	19	47	44	11	10	41	34	2	9	104	100	5	11	194	185	9	21	39	35	1	9	176	188	4	24	79	75	8	20	45	41
6	1	29	38	11	12	84	88	2	11	168	110	5	12	41	45	9	27	48	49	1	10	86	57	5	2	63	69	8	24	41	37
6	2	55	54	11	16	54	55	2	12	45	40	5	13	136	138	10	1	86	80	1	11	58	58	5	5	26	28	9	2	71	73
6	3	23	15	11	18	33	30	2	14	37	37	5	14	30	41	10	3	32	38	1	13	28	9	5	7	146	146	9	4	65	65
6	6	80	73	12	3	47	50	2	15	87	87	5	15	32	25	10	4	31	33	1	16	33	48	5	8	80	93	9	7	112	113
6	7	36	16	12	5	68	72	2	16	42	41	5	17	29	22	10	5	58	56	1	17	37	39	5	9	131	122	9	8	29	35
6	8	28	38	12	13	41	43	2	18	56	63	5	21	77	86	10	6	47	54	1	18	33	26	5	10	64	63	9	9	41	36
6	9	36	32	13	3	32	38	2	19	80	79	5	31	42	41	10	9	44	43	1	24	37	33	5	11	65	66	9	11	121	119
6	13	125	139	13	4	34	33	2	21	76	72	6	1	25	15	13	10	121	112	2	1	84	145	5	12	48	36	9	17	39	37
6	14	107	107	13	6	31	30	2	22	39	47	6	2	84	98	10	12	52	54	2	2	72	78	5	14	70	72	9	23	57	58
6	15	134	134	13	11	32	33	2	26	37	36	6	3	57	74	10	13	38	43	2	4	131	127	5	16	56	54	9	27	69	61
6	16	41	44	13	17	38	36	2	29	62	71	6	5	78	88	10	14	59	61	2	5	79	75	5	17	84	83	10	1	119	117
6	17	38	39	14	14	39	32	2	31	44	48	6	6	80	80	10	15	39	32	2	6	60	55	5	20	39	35	10	2	45	51
6	19	39	39					3	2	96	112	6	8	85	96	10	19	34	34	2	7	26	35	5	22	43	38	10	3	103	105
7	1	66	58					3	3	229	202	6	9	143	149	11	2	91	93	2	8	158	138	6	1	143	159	10	4	77	83
7	2	39	39					3	4	122	86	6	10	177	187	11	3	67	74	2	9	40	35	6	2	27	15	10	5	43	88
7	3	24																													

Table 4. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
10	8	62	51	2	25	73	79	7	8	38	42	13	2	56	56	3	8	92	72	7	5	68	67	13	1	49	50	3	4	149	99				
10	9	62	66	3	2	132	140	7	11	51	48	13	3	46	46	3	9	49	23	7	6	57	43	13	2	40	38	3	5	93	69				
10	10	108	103	3	4	58	38	7	11	24	27	13	4	38	39	3	11	84	91	7	10	44	46	13	3	52	46	3	6	32	8				
10	11	44	42	3	5	183	169	7	18	37	37	13	7	35	40	3	11	64	71	7	16	44	44	14	0	61	69	3	7	26	8				
10	12	32	27	3	6	71	74	7	19	63	60	13	9	36	33	3	12	57	57	7	17	30	25	14	4	31	34	3	8	108	121				
10	15	31	28	3	7	67	23	7	22	81	82	13	23	34	38	3	13	44	55	7	18	78	83	14	20	41	38	3	9	130	184				
10	24	39	44	3	8	155	166	7	24	40	46	14	4	38	40	3	18	95	101	7	22	113	111	15	2	46	41	3	10	42	25				
11	3	62	57	3	9	33	28	8	1	68	69	14	6	42	42	3	22	63	62	7	24	46	46	15	5	34	36	3	11	72	75				
11	6	89	97	3	10	75	80	8	2	77	77	14	7	36	34	4	0	137	75	8	0	161	170	16	1	47	44	3	12	66	69				
11	7	58	55	3	11	154	156	8	3	86	75	15	2	33	32	4	1	56	54	8	1	85	91	3	13	140	142	3	13	140	142				
11	8	65	73	3	14	76	72	8	4	156	163	15	3	38	42	4	2	42	8	8	2	37	27	3	14	130	125	3	14	130	125				
11	10	43	50	3	18	28	36	8	5	135	138	16	1	37	40	4	4	106	76	8	3	30	28	3	16	41	42	3	16	41	42				
11	26	42	43	4	1	33	57	8	6	45	46	16	5	47	41	4	6	65	78	8	4	56	59	8	6	156	137	3	17	42	55				
12	2	51	49	4	3	70	109	8	8	58	66	4	8	137	144	4	8	57	41	8	5	57	41	0	8	117	96	3	18	116	111				
12	3	57	58	4	4	262	272	8	9	77	76	4	9	44	34	4	9	44	34	8	6	48	52	0	10	90	91	3	21	48	33				
12	5	104	106	4	5	26	25	8	11	55	52	4	10	86	67	4	10	86	67	8	7	41	36	0	12	99	65	4	25	43	41				
12	9	94	92	4	6	76	97	8	14	41	39	4	11	89	88	4	11	89	88	8	14	28	19	0	14	90	92	4	0	310	258				
12	25	39	35	4	7	116	115	8	19	34	32	4	13	27	32	4	13	27	32	8	15	73	68	0	16	167	159	4	1	57	64				
13	5	37	43	4	8	52	45	8	21	75	76	4	14	27	26	4	14	27	26	8	16	42	44	0	18	88	80	4	2	161	152				
13	6	49	46	4	9	66	59	8	24	40	49	4	16	35	28	4	16	35	28	8	17	55	55	0	20	34	46	4	3	198	158				
13	7	42	45	4	10	27	4	8	25	58	64	4	18	30	35	4	18	30	35	8	19	64	71	0	22	44	34	4	4	206	170				
13	8	36	34	4	11	43	46	9	1	99	95	4	20	140	139	4	20	140	139	8	20	163	166	0	24	84	79	4	5	23	39				
14	8	34	35	4	12	73	67	9	3	162	172	5	1	85	83	5	1	85	83	8	21	96	95	0	26	76	75	4	6	170	165				
14	10	44	42	4	20	62	77	9	4	61	77	5	3	113	145	5	3	113	145	8	25	36	34	0	28	38	38	4	7	113	106				
16	9	47	46	4	24	46	59	9	7	145	147	5	4	147	140	5	4	147	140	9	1	117	122	1	2	36	15	4	8	39	36				
17	8	46	42	5	1	29	28	9	10	29	30	1	4	74	23	5	5	140	170	9	3	155	164	1	3	37	84	4	9	28	23				
H = -1				5	2	49	50	9	11	50	47	1	6	246	255	5	6	45	31	9	13	29	24	1	5	76	46	4	10	37	49				
				5	3	52	85	9	12	50	46	1	7	56	66	5	7	97	115	9	17	61	66	1	7	41	70	4	11	25	27				
				5	4	50	26	9	13	38	41	1	8	148	127	5	8	87	89	9	18	33	31	1	8	49	55	4	12	41	34				
				5	5	66	44	9	19	60	66	1	10	68	83	5	9	27	33	9	19	78	77	1	9	88	68	4	13	48	35				
0	6	31	11	5	7	59	57	9	21	36	32	1	11	71	65	5	13	31	21	9	21	106	102	1	10	76	111	4	14	87	94				
0	8	199	224	5	8	58	50	9	23	95	98	1	14	57	92	5	14	28	24	9	23	67	69	1	12	191	178	4	15	51	59				
0	10	30	45	5	9	27	22	10	1	13	39	1	16	63	101	5	16	30	35	10	0	110	113	1	13	142	155	4	16	164	168				
0	12	38	15	5	11	52	59	10	4	82	88	1	18	68	87	5	17	59	61	10	1	67	76	1	14	130	139	4	17	54	56				
0	16	57	53	5	12	81	98	10	5	94	99	1	19	48	53	5	19	85	87	10	2	38	45	1	15	59	46	4	20	55	55				
0	20	92	90	5	14	44	53	10	6	63	60	1	21	34	43	5	21	58	55	10	3	30	38	1	17	92	93	5	0	32	38				
1	24	126	125	5	20	51	48	10	7	28	22	1	24	58	71	5	23	42	45	10	4	53	54	1	18	55	54	5	2	114	102				
1	26	98	100	5	23	64	67	10	8	93	96	2	0	87	23	6	0	50	47	10	5	36	41	1	19	31	24	5	3	51	49				
1	4	268	207	6	1	52	83	10	12	49	48	2	3	75	25	6	1	23	38	10	8	30	18	1	27	34	34	5	4	28	9				
1	7	257	196	6	2	149	138	10	15	46	50	2	4	65	59	6	3	27	35	10	10	64	65	2	0	29	30	5	7	194	188				
1	9	283	204	6	3	101	95	10	20	65	63	2	5	268	279	6	4	21	34	10	16	66	67	2	1	52	102	5	8	88	73				
1	10	62	52	6	5	95	94	10	21	38	40	2	6	205	221	6	5	22	13	10	19	34	33	2	4	46	6	5	9	96	110				
1	11	97	87	6	6	79	78	10	24	48	55	2	7	65	74	6	7	39	44	10	20	93	89	2	5	140	146	5	10	47	60				
1	14	34	45	6	7	69	69	11	2	153	152	2	8	91	85	6	8	23	31	18	21	39	39	2	6	105	86	5	11	86	81				
2	1	315	354	6	8	22	24	11	3	29	22	2	10	66	93	6	9	105	104	11	1	44	48	2	7	111	77	5	12	61	50				
2	2	80	112	6	10	47	45	11	4	56	58	2	13	119	116	6	13	31	29	11	2	106	99	2	8	84	105	5	13	83	81				
2	3	324	229	6	14	29	28	11	6	85	78	2	15	36	42	6	14	34	35	11	4	74	70	2	9	24	8	5	14	33	22				
2	4	29	10	6	15	41	39	11	8	56	64	2	17	58	49	6	15	28	34	11	5	33	34	2	11	43	24	5	17	97	101				
2	6	33	24	6	19	44	49	11	22	56	58	2	19	128	136	6	16	58	50	11	12	31	31	2	15	222	226	5	19	75	77				
2	8	170	145	6	20	50	55	12	1	48	44	2	21	42	42	6	19	62	68	11	18	51	48	2	17	74	80	6	0	21	7				
2	9	169	153	7	2	107	98	12	3	33	42	3	1	38	53	6	20	50	59	11	22	58	50	2	19	98	96	6	1	69	98				
2	10	59	59	7	3	56	53	12	5	97	91	3	3	39	36	6	21	86	83	12	1	101	107	2	21	31	25	6	3	33	29				
2	12	120	116	7	4	99	90	12	8	35	34	3	4	342	287	6	25	43	44	12	5	40	39	2	23	55	55	6	4	73	51				
2	17	67	69	7	5	30	31	12	18	42	35	3	5	89	68	7	2	248	243	12	7	30	31	2	25	57	48	6	5	98	123				
2	21	89	84	7	6	69	83	13	1	42	44	3	6	109	73																				

Table 4. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
6	14	55	59	12	9	32	31	2	12	33	23	5	6	94	62	10	1	37	50	1	29	46	44	4	15	49	47	8	6	46	53				
6	15	99	109	12	11	44	40	2	13	33	43	5	9	36	34	10	5	35	38	2	1	22	24	4	16	33	35	8	7	50	58				
6	16	34	48	12	19	35	40	2	14	48	48	5	11	129	127	10	3	30	26	2	2	112	76	4	18	42	48	8	8	58	49				
6	17	41	41	13	10	41	40	2	15	249	235	5	12	86	77	10	10	89	88	2	3	71	45	4	20	63	61	8	9	71	75				
6	19	81	78	13	17	45	41	2	17	34	34	5	13	139	145	10	11	48	49	2	4	65	39	4	23	34	35	8	10	109	112				
6	21	32	31	13	19	44	48	2	18	75	71	5	15	55	47	10	14	44	45	2	5	229	173	4	26	83	81	8	11	106	97				
7	0	23	32	14	0	41	39	2	20	44	44	5	17	46	49	10	19	32	33	2	6	80	59	4	30	60	71	8	12	31	25				
7	2	52	75	14	14	42	39	2	21	63	63	5	22	31	34	11	2	81	80	2	7	69	76	5	0	47	50	8	19	57	53				
7	4	62	62	14	16	39	37	2	22	35	37	5	29	46	47	11	8	71	74	2	8	64	53	5	4	156	162	9	3	24	24				
7	6	83	75	15	1	39	34	2	24	49	48	6	0	41	57	11	12	52	54	2	9	55	62	5	5	38	45	9	4	42	39				
7	8	102	104	16	15	51	50	2	29	62	63	6	1	68	61	11	14	53	51	2	10	48	59	5	6	133	129	9	5	30	34				
7	9	26	24					2	31	55	55	6	2	126	128	11	18	40	41	2	11	217	209	5	7	208	206	9	7	79	76				
7	10	50	56					3	0	194	141	6	3	96	87	12	1	43	43	2	13	25	35	5	8	89	89	9	9	81	73				
7	11	46	39					3	1	200	263	6	4	66	54	12	4	33	37	2	14	115	116	5	9	198	207	9	10	30	33				
7	12	61	62					3	3	144	123	6	5	42	36	12	11	68	68	2	15	91	86	5	11	49	55	9	22	33	31				
7	14	45	49					3	4	119	137	6	7	125	135	12	15	55	46	2	16	26	26	5	13	58	56	9	27	48	46				
7	16	46	47					3	5	54	74	6	9	153	160	13	3	45	43	2	17	78	77	5	15	28	24	10	0	38	41				
7	18	121	117					3	6	51	79	6	10	92	94	13	9	43	37	2	18	37	35	5	16	29	21	10	1	32	32				
8	0	56	57					3	7	117	110	6	11	109	125	13	10	36	33	2	19	38	43	5	22	49	52	10	2	29	27				
8	1	45	61					3	9	165	150	6	14	67	61	13	13	53	54	2	21	51	52	5	27	46	46	18	3	31	27				
8	2	52	56					3	10	71	64	6	15	51	61	13	14	34	35	2	22	57	56	5	29	66	64	18	5	47	41				
8	3	72	74					3	12	151	159	6	16	45	44	14	7	33	28	2	25	86	88	6	0	69	81	10	6	55	54				
8	11	36	43					3	13	135	143	6	21	40	40	14	10	62	57	2	27	52	53	6	1	202	202	10	7	29	26				
8	14	66	65					3	14	168	170	6	22	40	39	14	12	39	37	2	29	47	48	6	2	83	42	10	10	67	83				
8	15	73	68					3	15	48	46	6	25	36	34	15	14	42	39	2	31	48	45	6	3	90	61	10	11	57	59				
8	16	42	42					3	16	42	53	6	31	40	42	16	11	46	44	3	0	128	142	6	5	108	119	10	16	31	28				
8	17	39	43					3	18	41	49	7	0	25	42					3	1	195	182	6	6	96	92	11	2	39	36				
8	19	41	43					3	20	54	58	7	1	72	81					3	2	36	47	6	7	64	56	11	4	57	68				
8	20	74	75					3	21	35	42	7	5	83	99					3	3	91	97	6	9	169	167	11	7	43	48				
9	0	34	36					3	24	36	40	7	6	45	50					0	0	42	66	3	5	195	162	11	8	61	61				
9	2	27	17					3	25	37	38	7	8	75	82					0	2	188	30	3	6	122	132	11	10	34	35				
9	4	32	31					3	26	61	60	7	9	34	34					0	4	114	144	3	8	158	173	11	13	44	47				
9	7	33	35					4	1	97	47	7	12	137	146					3	6	177	182	3	9	111	119	12	0	78	74				
9	13	107	182					4	1	76	77	7	14	103	102					0	8	77	82	3	10	111	112	12	1	58	56				
9	17	85	85					4	2	176	186	7	15	51	43					0	10	142	148	3	11	74	78	12	7	72	77				
9	18	44	39					4	3	58	75	7	22	38	37					0	14	145	132	3	12	131	131	12	9	51	46				
9	19	60	57					4	4	21	12	7	25	33	30					0	18	58	52	3	13	73	77	12	10	31	36				
9	27	37	36					4	5	21	49	7	28	40	38					0	22	36	28	3	14	103	103	12	11	61	57				
10	0	95	91					4	6	37	46	8	1	28	9					0	24	44	45	3	15	59	53	13	7	63	61				
10	1	72	69					4	7	100	74	8	7	56	57					0	26	49	44	3	16	65	66	13	8	64	67				
10	2	63	64					4	8	34	37	8	8	52	57					0	30	48	48	3	17	77	79	13	9	78	78				
10	4	26	34					4	9	51	51	8	10	47	54					1	0	26	20	3	18	37	39	13	12	35	35				
10	8	31	37					4	10	173	157	8	11	89	96					1	1	29	17	3	21	51	50	14	6	56	53				
10	12	78	83					4	11	59	55	8	12	41	52					1	2	21	13	3	22	33	39	14	14	88	79				
10	14	50	51					4	12	93	103	8	13	41	45					1	3	208	148	3	28	86	91	15	8	38	42				
10	16	53	51					4	14	64	72	8	14	44	40					1	4	165	129	4	0	78	93	15	7	39	38				
10	19	35	36					4	15	40	34	8	15	62	58					1	5	35	49	4	2	34	45	15	8	39	39				
10	20	40	42					4	16	119	119	8	20	42	46					1	6	42	54	4	3	74	69	15	9	45	44				
11	0	77	79					4	19	37	31	9	3	46	44					1	7	47	52	4	4	69	80	16	5	36	48				
11	1	54	50					4	20	28	21	9	7	58	64					1	8	221	207	4	6	99	108	16	11	37	31				
11	6	32	33					4	23	38	45	9	8	38	39					1	9	191	173	4	7	24	20	17	8	46	37				
11	12	45	48					4	30	54	56	9	9	69	70					1	11	127	112	4	9	108	115								
11	14	42	45					5	1	73	54	9	11	49	48					1	12	125	136	4	10	178	155								
11	18	78	70					5	1	82	85	9	13	130	129					1	13	148	156	4	11	129	123								
12	1	55	55					5	4	154	171	9	15																						

Table 4. (Continued)

K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC
0	4	162	138	3	23	53	58	7	1	40	56	11	7	47	46	1	24	60	66	4	19	37	35	8	16	41	37				
0	6	105	90	3	24	86	95	7	3	25	27	11	8	85	91	1	25	52	47	4	20	93	93	8	19	40	41				
0	8	79	65	3	28	69	66	7	4	127	123	11	24	51	56	2	0	28	33	4	21	71	67	8	21	42	39	0	0	158	161
0	13	37	49	4	0	38	33	7	5	24	20	12	2	31	36	2	1	270	257	4	22	77	74	8	22	38	35	0	2	24	11
0	16	136	135	4	1	117	147	7	6	77	71	12	4	33	34	2	3	77	44	4	24	44	41	9	0	26	24	0	4	29	34
0	22	37	26	4	2	65	68	7	7	30	26	12	5	85	86	2	4	29	30	5	1	26	35	9	3	121	127	0	6	52	64
0	26	47	44	4	3	198	176	7	8	98	103	12	6	48	47	2	5	211	181	5	2	28	16	9	4	29	25	0	12	78	84
1	1	98	43	4	4	121	134	7	9	66	75	12	7	88	85	2	6	41	23	5	3	221	221	9	5	59	59	0	16	143	146
1	2	89	76	4	6	185	195	7	10	29	34	12	9	86	90	2	8	91	85	5	4	98	95	9	6	83	80	0	18	42	46
1	3	108	143	4	7	97	101	7	11	31	24	12	14	40	35	2	9	72	79	5	5	121	115	9	8	20	24	0	20	119	112
1	4	136	146	4	10	105	95	7	12	97	100	12	21	45	43	2	10	93	69	5	6	95	97	9	10	30	36	0	22	63	68
1	5	87	90	4	11	37	45	7	13	31	34	13	3	60	66	2	11	32	14	5	7	34	37	9	11	44	42	1	1	32	20
1	7	63	84	4	12	51	48	7	19	33	32	13	4	36	32	2	12	35	41	5	11	70	64	9	12	54	64	1	3	43	29
1	8	134	127	4	14	65	61	7	20	33	25	13	7	87	87	2	14	46	37	5	13	49	46	9	13	82	82	1	4	37	45
1	9	119	110	4	15	58	56	7	24	39	39	13	8	57	58	2	15	34	29	5	15	30	35	9	15	58	59	1	7	22	35
1	10	34	40	4	18	34	39	7	28	44	38	13	9	46	40	2	16	32	30	5	19	82	79	9	19	37	36	1	8	39	32
1	13	37	6	4	22	86	80	8	1	59	60	13	10	43	42	2	17	31	25	5	23	70	76	9	23	42	45	1	10	26	32
1	15	37	31	4	24	46	50	8	2	24	33	14	6	104	98	2	18	35	29	6	0	157	141	10	0	85	79	1	11	60	61
1	16	85	91	4	25	41	42	8	4	39	40	14	15	40	38	2	20	49	44	6	1	208	202	10	1	73	76	1	12	30	35
1	17	57	58	4	26	80	87	8	5	67	72	15	3	36	28	2	21	121	120	6	2	151	152	10	2	70	67	1	14	89	84
1	21	46	46	4	27	39	36	8	6	89	103	15	7	41	36	2	25	46	46	6	3	78	71	10	3	59	57	1	15	182	118
1	23	33	37	5	0	77	79	8	7	52	62	15	8	41	44	3	0	180	182	6	5	123	123	10	6	58	57	1	17	45	45
1	28	41	38	5	1	33	47	8	8	48	54	16	5	61	53	3	1	29	44	6	6	46	49	10	11	36	34	1	18	83	86
2	0	30	61	5	2	145	143	8	9	45	49	16	7	38	38	3	2	160	144	6	7	76	71	10	12	51	55	1	19	92	98
2	1	37	37	5	3	124	127	8	12	38	46	17	4	43	36	3	3	39	31	6	9	119	106	10	13	37	37	1	20	46	51
2	2	88	55	5	4	52	49	8	13	30	40					3	4	151	152	6	10	46	54	10	18	54	54	1	21	31	33
2	4	45	29	5	5	79	78	8	14	35	34					3	5	171	156	6	11	84	89	10	22	35	37	2	1	185	186
2	5	305	258	5	6	33	25	8	15	58	58					3	6	36	10	6	13	26	29	11	0	51	48	2	2	47	43
2	6	90	75	5	7	176	174	8	16	47	50					3	7	24	19	6	16	54	57	11	2	91	82	2	3	71	51
2	7	149	124	5	8	99	117	8	18	46	39					3	8	63	55	6	18	58	57	11	3	29	21	2	4	59	41
2	8	119	124	5	9	147	153	8	25	37	37					3	9	37	57	6	21	40	35	11	4	80	81	2	5	71	71
2	10	41	59	5	10	49	43	8	26	40	35					3	12	32	33	6	22	45	43	11	7	47	45	2	7	112	115
2	11	64	76	5	11	24	20	9	0	39	39					3	13	43	39	6	26	40	38	11	10	34	39	2	8	46	53
2	13	26	14	5	13	35	33	9	3	62	60					3	14	30	31	7	0	103	125	11	11	57	54	2	9	35	44
2	14	37	38	5	15	55	53	9	4	51	49					3	15	41	43	7	2	146	158	11	12	54	49	2	10	30	26
2	15	82	72	5	19	47	43	9	5	40	33					3	17	71	66	7	3	60	59	11	19	35	30	2	12	58	67
2	17	27	32	5	23	59	60	9	7	33	42					3	18	69	73	7	4	214	213	11	23	41	37	2	14	73	69
2	21	59	61	5	27	57	61	9	9	54	56					3	19	32	33	7	7	28	24	12	0	52	55	2	15	96	97
2	23	46	40	5	29	38	41	9	16	43	41					3	20	45	40	7	10	44	53	12	1	85	97	2	16	43	44
2	25	72	71	6	0	69	82	9	11	38	31					3	22	86	83	7	12	93	90	12	5	93	93	2	17	83	88
2	26	39	39	6	1	55	55	9	23	51	52					3	23	34	33	7	14	52	54	12	8	34	35	2	18	42	45
2	27	40	38	6	2	133	118	10	0	43	34					3	24	64	73	7	15	28	27	12	10	65	61	2	19	45	42
3	0	184	178	6	3	23	27	10	2	40	40					4	1	212	218	7	17	51	47	12	21	70	68	2	21	119	117
3	1	64	91	6	4	29	17	10	4	29	31					4	1	73	82	7	18	35	42	13	0	40	41	3	8	22	20
3	2	102	81	6	5	159	156	10	5	45	40					4	1	93	37	7	24	43	42	13	3	67	61	3	1	36	38
3	4	143	149	6	6	97	94	10	6	89	92					4	4	43	48	8	0	59	55	13	4	56	56	3	2	98	84
3	5	56	62	6	7	138	128	10	7	72	76					4	5	36	35	8	1	126	124	13	5	49	53	3	5	28	46
3	6	51	49	6	9	70	70	10	10	41	41					4	6	170	182	8	2	89	94	13	13	33	36	3	6	53	57
3	7	76	64	6	10	44	43	10	13	32	31					4	7	26	28	8	3	101	104	13	19	43	45	3	8	58	48
3	8	231	211	6	14	75	67	10	16	33	34					4	8	59	59	8	7	32	24	13	20	38	29	3	10	47	33
3	10	149	149	6	18	29	25	10	26	55	52					4	9	27	16	8	8	53	44	14	6	83	84	3	11	50	45
3	11	38	31	6	21	37	39	11	1	32	38					4	10	89	88	8	9	51	60	15	3	36	30	3	13	62	68
3	12	58	48	6	25	48	44	11	2	41	44					4	11	60	62	8	10	72	82	15	4	43	44	3	14	114	108
3	13	69	58	6	26	41	38	11	3	30	30					4	12	64	68	8	11	66	66	16	1	47	47	3	17	58	68
3	14	66	55	6	27	38	38	11	4	73	72					4	13	52	47	8	12	42	42					3	18	184	184
3	22	58	60	7	0	36	35	11	6	37	39					4	17	57	61	8	13	68	21					3	19	54	55

Table 4. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
3	20	79	86	7	13	37	40	0	18	71	64	5	13	161	163	11	18	41	36	3	8	93	89	8	2	62	64	1	28	35	36	1	28	35	36
3	24	35	30	7	11	43	38	1	1	71	71	5	14	29	34	12	1	45	46	3	9	54	59	8	10	52	50	1	25	48	53	1	25	48	53
4	0	179	202	7	17	34	29	1	1	34	26	5	15	110	109	12	11	40	42	3	10	114	114	8	11	95	95	1	29	39	40	1	29	39	40
4	1	41	44	7	10	67	61	1	2	75	67	5	17	52	54	12	13	43	49	3	12	59	57	8	12	77	73	2	0	54	58	2	0	54	58
4	2	83	88	7	21	42	40	1	7	39	42	5	19	38	38	12	15	35	26	3	13	132	135	8	13	47	53	2	1	55	53	2	1	55	53
4	3	34	37	8	0	79	83	1	8	55	59	6	0	37	36	12	17	52	52	3	14	119	121	8	15	59	56	2	7	114	114	2	7	114	114
4	6	67	77	8	1	115	119	1	10	34	38	6	1	79	79	13	13	51	54	3	16	47	45	8	16	35	43	2	11	87	89	2	11	87	89
4	7	50	37	8	2	73	81	1	11	34	38	6	3	75	71	13	15	48	48	3	19	37	36	9	1	63	68	2	13	27	21	2	13	27	21
4	13	53	58	8	5	69	69	1	13	104	96	6	5	87	77	14	12	45	47	3	30	41	41	9	3	53	52	2	17	67	45	2	17	67	45
4	15	53	55	8	12	51	54	1	14	108	110	6	7	51	59	14	16	47	47	4	0	29	14	9	5	34	39	2	16	30	27	2	16	30	27
4	16	78	88	8	14	48	52	1	15	89	82	6	11	117	122	15	14	43	44	4	1	23	29	9	6	50	49	2	25	37	31	2	25	37	31
4	17	57	58	8	16	73	79	1	17	40	43	6	12	91	99					4	2	43	41	9	9	91	94	2	27	74	72	2	27	74	72
4	18	36	48	8	17	55	58	2	1	28	32	6	13	70	74					4	3	74	84	9	13	67	64	3	1	46	53	3	1	46	53
4	20	110	137	8	18	55	58	2	3	61	67	6	15	81	87					4	4	47	38	9	15	64	71	3	4	57	47	3	4	57	47
4	22	44	44	9	1	34	31	2	4	74	68	6	16	49	47					4	5	92	81	9	17	34	32	3	5	55	61	3	5	55	61
5	1	36	36	9	2	51	47	2	5	23	25	6	17	80	81					4	6	68	60	10	1	44	43	3	6	27	27	3	6	27	27
5	3	108	112	9	3	65	66	2	6	43	33	6	18	39	38					4	8	92	88	10	1	29	22	3	8	132	125	3	8	132	125
5	4	57	65	9	17	50	57	2	8	47	51	7	1	46	47					4	9	29	39	10	2	36	36	3	9	124	123	3	9	124	123
5	5	28	19	9	19	77	81	2	9	33	28	7	2	28	37					4	10	104	104	10	3	34	32	3	10	113	116	3	10	113	116
5	6	31	22	10	0	81	90	2	10	64	73	7	3	59	68					4	11	95	99	10	4	29	38	3	11	51	47	3	11	51	47
5	7	76	58	10	1	38	29	2	11	112	114	7	4	66	70					4	12	138	134	10	10	56	60	3	12	34	34	3	12	34	34
5	8	52	55	10	2	54	53	2	13	66	68	7	7	30	36					4	13	43	42	10	11	36	31	3	18	49	93	3	18	49	93
5	9	91	85	10	4	42	43	2	15	105	106	7	10	69	69					4	16	68	62	10	12	55	56	3	21	32	31	3	21	32	31
5	10	56	49	10	9	38	32	2	17	119	118	7	12	43	35					4	19	38	27	11	4	35	28	3	24	42	42	3	24	42	42
5	13	36	31	10	13	39	45	3	1	48	34	7	14	156	148					4	22	32	29	11	6	34	37	4	4	54	55	4	4	54	55
5	14	37	37	10	15	36	45	3	1	27	46	7	16	36	25					4	26	45	41	11	10	33	26	4	5	39	31	4	5	39	31
5	15	61	64	10	16	55	53	3	2	23	18	7	18	43	46					5	3	68	70	11	14	49	44	4	6	147	149	4	6	147	149
5	17	61	61	10	22	35	37	3	3	74	76	7	21	48	50					5	4	33	37	11	16	47	46	4	7	187	113	4	7	187	113
5	18	32	37	11	0	63	61	3	8	79	76	8	0	38	45					5	5	35	32	12	11	46	41	4	8	99	109	4	8	99	109
5	19	78	72	11	3	48	53	3	10	50	46	8	6	27	28					5	7	55	58	13	9	36	34	4	18	97	108	4	18	97	108
5	21	47	45	11	8	58	57	3	12	68	65	8	8	40	38					5	9	175	177	14	12	48	48	4	11	57	49	4	11	57	49
5	23	36	36	11	15	34	40	3	13	104	107	8	12	41	44					5	11	29	36					4	12	61	59	4	12	61	59
6	0	117	99	11	16	34	36	3	14	160	166	8	13	39	40					5	12	32	32					4	15	45	45	4	15	45	45
6	1	221	218	11	18	71	73	3	15	41	40	8	15	60	58					5	13	108	116					4	19	39	35	4	19	39	35
6	2	132	125	11	20	41	42	3	16	34	35	8	16	61	58					5	15	63	64	0	0	73	67	4	26	53	53	4	26	53	53
6	3	43	42	12	7	37	41	3	18	42	42	8	18	41	42					5	29	41	46	0	4	35	32	4	28	36	35	4	28	36	35
6	5	68	62	12	15	48	40	3	19	30	35	9	1	31	28					6	0	74	72	0	10	59	60	5	0	40	41	5	0	40	41
6	6	39	40	12	17	48	44	4	0	82	94	9	9	29	34					6	1	92	84	0	12	65	62	5	2	25	18	5	2	25	18
6	7	54	51	12	21	46	44	4	1	47	54	9	11	35	33					6	2	66	59	0	16	53	50	5	3	58	66	5	3	58	66
6	8	75	78	13	7	40	40	4	3	97	98	9	13	88	86					6	3	49	54	0	22	50	49	5	4	43	41	5	4	43	41
6	9	65	55	13	9	44	42	4	4	63	50	9	15	92	91					6	7	86	83	0	26	87	89	5	5	118	111	5	5	118	111
6	10	28	33	13	17	47	52	4	5	61	66	9	19	34	28					6	8	68	62	0	28	56	56	5	7	89	90	5	7	89	90
6	12	51	46	13	19	59	61	4	6	43	56	9	23	35	36					6	10	57	57	1	1	26	32	5	9	160	161	5	9	160	161
6	13	30	27	14	2	36	28	4	7	27	36	10	1	37	39					6	11	111	121	1	2	59	59	5	10	61	49	5	10	61	49
6	14	34	38	14	16	57	56	4	10	161	170	10	7	50	45					6	12	79	74	1	3	28	29	5	13	33	36	5	13	33	36
6	15	35	38	15	19	37	36	4	12	152	161	10	12	47	41					6	14	47	47	1	4	75	80	5	25	56	52	5	25	56	52
6	16	44	45	16	1	34	35	4	13	47	47	10	15	45	43					6	15	63	65	1	5	37	44	6	3	49	54	6	3	49	54
6	17	53	50					4	14	41	40	10	16	51	56					6	16	46	45	1	6	34	36	6	4	69	72	6	4	69	72
6	21	32	33					4	16	144	145	10	17	41	46					6	17	41	41	1	8	29	28	6	5	63	65	6	5	63	65
7	0	165	171					4	18	63	67	10	18	41	41					7	0	57	55	1	9	84	84	6	6	89	92	6	6	89	92
7	1	39	35					5	1	53	48	11	2	29	27					7	8	66	72	1	10	66	67	6	7	118	128	6	7	118	128
7																																			

Table 4. (Continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
6	25	56	46	1	13	79	75	5	11	29	34	15	4	44	44	5	9	48	46	4	3	110	98	7	3	48	45	5	4	34	35	5	4	34	35
6	27	44	48	1	14	85	81	5	23	50	50					5	15	33	29	0	10	61	60	7	4	42	38	5	7	39	39	5	7	39	39
7	4	65	67	1	15	58	55	5	25	64	64					5	15	44	40	0	12	81	91	7	7	52	58	5	10	33	30	5	10	33	30
7	8	80	82	1	16	46	51	6	1	40	36					5	19	57	60	0	16	47	50	7	14	40	42	5	11	39	39	5	11	39	39
7	9	28	27	1	18	39	38	6	1	72	77					5	21	61	56	0	18	100	96	7	16	72	73	5	15	41	35	5	15	41	35
7	10	66	68	1	19	54	54	6	2	69	72					5	23	40	35	1	0	87	91	7	20	70	72	6	1	33	32	6	1	33	32
7	12	45	53	1	23	53	53	6	3	114	120					6	1	109	126	1	3	42	34	6	1	38	40	6	3	39	42	6	3	39	42
7	14	36	40	1	24	63	64	6	6	65	61					0	10	32	30	1	5	30	25	6	4	40	44	6	5	31	37	6	5	31	37
7	24	63	61	1	25	51	51	6	7	81	93					0	12	49	51	6	3	67	69	6	6	43	44	7	4	44	50	7	4	44	50
8	5	43	42	2	0	41	35	6	10	65	66					0	16	39	36	1	6	29	24	8	6	43	45	7	10	34	32	7	10	34	32
8	6	84	77	2	1	97	96	6	21	45	44					0	22	53	53	1	9	47	46	8	13	47	45	7	14	49	48	7	14	49	48
8	7	106	98	2	2	25	24	6	22	39	39					1	0	92	97	1	12	31	30	8	18	52	55	7	16	49	43	7	16	49	43
8	8	51	48	2	3	85	86	6	23	58	54					1	1	79	79	6	14	33	30	9	1	64	67	8	12	44	42	8	12	44	42
8	11	40	75	2	5	74	74	7	2	46	50					1	3	54	54	1	14	69	65	9	2	43	46	8	13	44	39	8	13	44	39
8	13	32	33	2	7	63	66	7	4	134	134					6	22	65	63	1	15	80	78	9	15	88	86	8	14	51	45	8	14	51	45
9	0	44	52	2	13	42	40	7	5	35	38					1	9	42	37	1	17	34	34	9	19	63	59	9	15	76	79	9	15	76	79
9	2	67	59	2	18	34	36	7	6	42	49					1	12	32	31	2	2	42	47	10	16	44	46	10	11	35	31	10	11	35	31
9	4	32	23	2	21	45	47	7	7	45	44					1	17	49	43	2	12	38	39	11	0	51	48	10	12	69	66	10	12	69	66
9	5	78	82	2	23	53	51	7	8	60	58					1	18	39	37	2	13	82	79	11	14	52	52	10	13	39	38	10	13	39	38
9	6	34	34	2	25	51	51	7	12	41	33					1	19	55	56	2	14	65	68					10	16	40	38	10	16	40	38
9	7	35	34	2	27	44	48	7	20	40	41					1	20	62	63	2	15	35	40					11	10	52	52	11	10	52	52
9	9	61	61	3	0	99	100	7	24	70	71					2	1	167	171	7	18	37	35					11	14	41	42	11	14	41	42
9	12	34	31	3	1	40	39	8	0	45	45					2	3	111	119	7	20	89	82					11	16	40	38	11	16	40	38
10	1	30	36	3	3	25	26	8	1	42	34					2	13	41	35	7	24	40	41					12	11	41	42	12	11	41	42
10	3	44	44	3	4	130	146	8	2	67	59					8	1	36	39	8	2	73	75					12	13	41	42	12	13	41	42
10	4	36	40	3	5	59	67	8	3	56	57					8	3	51	54	3	10	30	27					12	14	41	42	12	14	41	42
10	5	45	44	3	6	50	50	8	5	29	32					8	4	40	44	3	12	55	58					12	15	41	42	12	15	41	42
10	6	72	75	3	8	49	52	8	6	55	58					8	9	35	30	3	14	71	67					12	16	41	42	12	16	41	42
10	7	33	39	3	10	38	41	8	7	58	58					8	16	35	39	3	16	46	44					12	17	41	42	12	17	41	42
10	8	35	36	3	13	33	31	8	15	39	34					8	17	56	54	4	2	41	37					12	18	41	42	12	18	41	42
11	0	38	39	3	14	83	82	8	22	52	52					8	18	42	41	4	6	98	95					12	19	41	42	12	19	41	42
11	1	63	70	3	15	45	44	8	23	42	39					8	21	48	48	4	8	84	82					12	20	41	42	12	20	41	42
11	4	41	43	3	17	38	34	9	0	34	24					8	22	49	50	4	12	30	26					12	21	41	42	12	21	41	42
11	5	55	58	3	24	90	88	9	2	57	53					9	1	61	57	4	13	76	71					12	22	41	42	12	22	41	42
11	8	38	45	4	1	31	25	9	3	91	96					9	5	53	54	4	14	53	56					12	23	41	42	12	23	41	42
12	4	43	47	4	2	113	111	9	5	78	75					9	5	53	54	5	1	34	29					12	24	41	42	12	24	41	42
12	7	44	41	4	3	73	76	9	7	41	39					9	19	65	65	5	3	30	29					12	25	41	42	12	25	41	42
12	11	38	37	4	4	49	50	9	13	38	36					10	2	50	53	5	5	50	49					12	26	41	42	12	26	41	42
13	5	37	35	4	5	29	26	9	19	43	40					10	3	35	37	5	10	31	29					12	27	41	42	12	27	41	42
14	6	58	58	4	6	131	139	10	1	47	55					10	6	34	34	5	11	65	63					12	28	41	42	12	28	41	42
14	8	43	41	4	7	71	68	10	2	78	85					10	15	34	33	5	12	44	40					12	29	41	42	12	29	41	42
				4	8	69	72	10	3	32	33					10	16	38	36	5	13	40	37					12	30	41	42	12	30	41	42
				4	12	32	32	10	6	52	58					10	18	38	40	5	15	45	48					12	31	41	42	12	31	41	42
				4	13	59	59	11	0	35	39					11	0	77	74	5	19	48	47					12	32	41	42	12	32	41	42
				4	19	35	33	11	1	44	46					11	3	35	34	6	1	72	32					12	33	41	42	12	33	41	42
				4	22	59	59	11	4	67	69					11	4	46	43	6	5	64	67					12	34	41	42	12	34	41	42
				4	23	34	34	11	8	34	37					12	1	56	56	6	6	37	36					12	35	41	42	12	35	41	42
				4	26	45	50	12	1	48	45					13	1	45	41	6	7	53	55					12	36	41	42	12	36	41	42
				5	0	41	48	12	3	72	75					14	2	66	62	6	9	31	28					12	37	41	42	12	37	41	42
				5	1	75	78	12	7	55	53					15	0	45	47	6	13	33	43					12	38	41	42	12	38	41	42
				5	3	95	96	13	0	43	41					6	14	37	36	6	14	37	36					12	39	41	42	12	39	41	42
				5	4	36	38	13	3	37	36					6	17	44	46	6	17	44	46					12	40	41	42	12	40	41	42
				5	5	151	152	13	4	51	52					6	18	46	45	6	18	46	45					12	41	41	42	12	41	41	42

Table 4. (Continued)

[illegible]

CHAPTER III

RESULTS AND DISCUSSION

The structure of $[\text{Co}_3(\text{Dma})_6](\text{ClO}_4)_2$ is shown in Figures 4 and 5 (see Figure 6 for the system of numbering). Bond distances and bond angles are given in Tables 5 and 6, respectively. The structure consists of linear trinuclear cations and discrete perchlorate anions. Each of the terminal cobalt atoms is octahedrally coordinated by three chelate ligands through the oxime and imine nitrogen atoms. The central cobalt is octahedrally coordinated by the six oxime oxygens.

In order to balance charges, it is necessary for two of the cobalt ions to be trivalent and one to be divalent. Charge assignments at the terminal and central cobalts can be made on the basis of bond distances. Co-N distances for the terminal cobalt atoms are between 1.89 - 2.00 Å and Co-O distances for the central cobalt are between 2.10 - 2.12 Å. Reported Co(II)-N distances lie between 2.11 - 2.241 Å^{11,37} and Co(III)-N distances between 1.88 - 2.02 Å.^{11,12,37} Co(II)-O distances of 1.99 - 2.225 Å have been observed^{8,9,10} and Co(III)-O distances of 1.83 - 1.98 Å.^{10,11,12} Comparison of Co-N distances indicates that the terminal cobalt ions can be assigned as cobalt(III) and comparison of Co-O

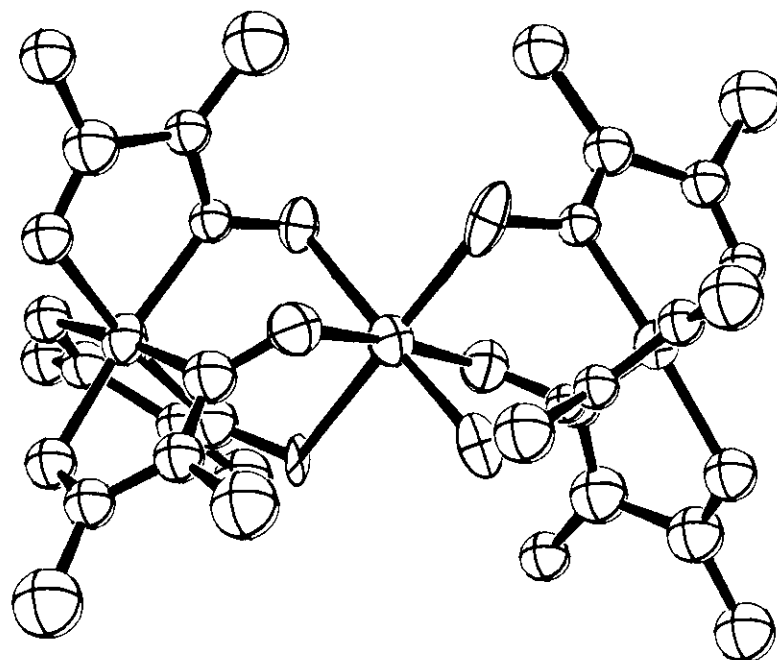


Figure 4. A Perspective Drawing of the Structure
of $[\text{Co}_3(\text{Dma})_6](\text{ClO}_4)_2$ (Phenyl Rings and
Perchlorates omitted)

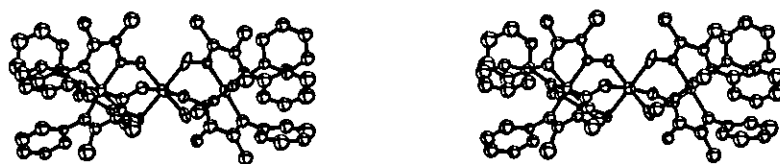


Figure 5. A Stereo View of $[\text{Co}_3(\text{Dma})_6](\text{ClO}_4)_2$
(Perchlorates omitted)

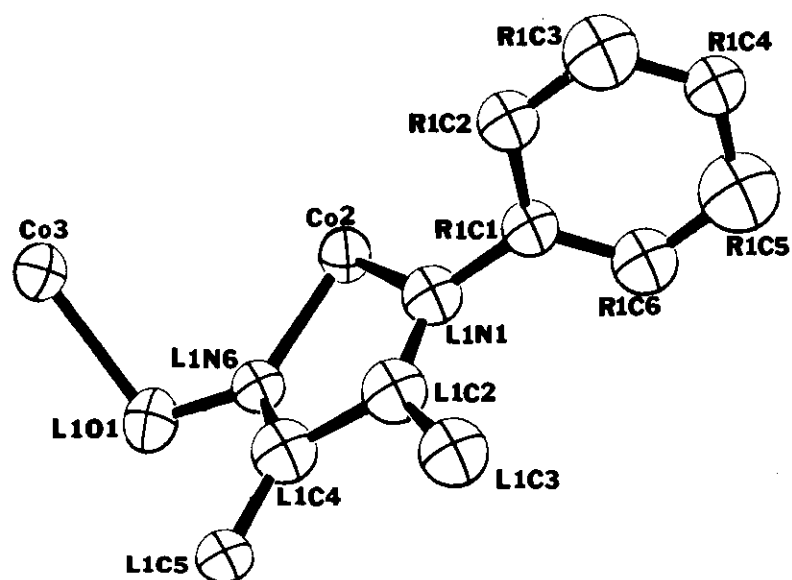


Figure 6. System of Numbering Used for
 $[\text{Co}_3(\text{Dma})_6](\text{ClO}_4)_2$

Table 5. Interatomic Distances for $[\text{Co}_3(\text{Dma})_6](\text{ClO}_4)_2$

Atoms	Distances (Å)	Atoms	Distances (Å)
Co1-Co3	3.453(4)	L2N1-L2C2	1.31(2)
Co2-Co3	3.455(4)	L2C2-L2C3	1.52(2)
Co1-L4N1	1.96(1)	L2C2-L2C4	1.45(2)
Co1-L4N6	1.89(1)	L2C4-L2C5	1.52(2)
Co1-L5N1	1.98(1)	L2C4-L2N6	1.29(2)
Co1-L5N6	1.89(1)	L2N6-L2O1	1.32(1)
Co1-L6N1	1.97(1)	L3N1-L3C2	1.28(2)
Co1-L6N6	1.89(1)	L3C2-L3C3	1.51(3)
Co2-L1N1	2.00(1)	L3C2-L3C4	1.46(2)
Co2-L1N6	1.91(1)	L3C4-L3C5	1.55(2)
Co2-L2N1	1.97(1)	L3C4-L3N6	1.28(2)
Co2-L2N6	1.90(1)	L3N6-L3O1	1.31(1)
Co2-L3N1	1.97(1)	L4N1-L4C2	1.33(2)
Co2-L3N6	1.91(1)	L4C2-L4C3	1.53(2)
Co3-L1O1	2.12(1)	L4C2-L4C4	1.42(2)
Co3-L2O1	2.117(9)	L4C4-L4C5	1.52(2)
Co3-L3O1	2.12(1)	L4C4-L4N6	1.32(2)
Co3-L4O1	2.12(1)	L4N6-L4O1	1.31(1)
Co3-L5O1	2.10(1)	L5N1-L5C2	1.28(2)
Co3-L6O1	2.109(9)	L5C2-L5C3	1.54(3)
L1N1-L1C2	1.28(2)	L5C2-L5C4	1.45(2)
L1C2-L1C3	1.50(3)	L5C4-L5C5	1.53(2)
L1C2-L1C4	1.48(2)	L5C4-L5N6	1.31(2)
L1C4-L1C5	1.48(3)	L5N6-L5O1	1.32(1)
L1C4-L1N6	1.32(2)	L6N1-L6C2	1.27(2)
L1N6-L1O1	1.31(1)	L6C2-L6C3	1.54(3)
L6C2-L6C4	1.44(2)		
L6C4-L6C5	1.50(2)		
L6C4-L6N6	1.32(2)		
L6N6-L6O1	1.32(1)		

Table 6. Interatomic Angles for $[\text{Co}_3(\text{Dma})_6](\text{ClO}_4)_2$

Atoms	Degrees	Atoms	Degrees
L4N1-Co1-L4N6	81.6(5)	L2N1-Co2-L3N6	171.3(5)
L4N1-Co1-L5N1	97.1(5)	L2N6-Co2-L3N1	91.5(5)
L4N1-Co1-L5N6	171.2(5)	L2N6-Co2-L3N6	90.3(5)
L4N1-Co1-L6N1	95.9(5)	L3N1-Co2-L3N6	81.0(5)
L4N1-Co1-L6N6	92.3(5)	L1O1-Co3-L2O1	89.6(4)
L4N6-Co1-L5N1	92.2(5)	L1O1-Co3-L3O1	89.4(4)
L4N6-Co1-L5N6	89.8(5)	L1O1-Co3-L4O1	175.7(4)
L4N6-Co1-L6N1	171.8(5)	L1O1-Co3-L5O1	94.8(4)
L4N6-Co1-L6N6	90.9(5)	L1O1-Co3-L6O1	87.3(4)
L5N1-Co1-L5N6	81.3(5)	L2O1-Co3-L3O1	91.0(4)
L5N1-Co1-L6N1	95.9(5)	L2O1-Co3-L4O1	92.3(4)
L5N1-Co1-L6N6	170.5(4)	L2O1-Co3-L5O1	86.3(4)
L5N6-Co1-L6N1	92.8(5)	L2O1-Co3-L6O1	174.6(4)
L5N6-Co1-L6N6	89.7(5)	L3O1-Co3-L4O1	86.8(4)
L6N1-Co1-L6N6	81.3(5)	L3O1-Co3-L5O1	175.0(4)
L1N1-Co2-L1N6	81.3(5)	L3O1-Co3-L6O1	93.3(4)
L1N1-Co2-L2N1	97.4(5)	L4O1-Co3-L5O1	89.2(4)
L1N1-Co2-L2N6	171.1(5)	L4O1-Co3-L6O1	91.1(4)
L1N1-Co2-L3N1	97.4(5)	L5O1-Co3-L6O1	89.6(4)
L1N1-Co2-L3N6	91.2(5)	Co3-L1O1-L1N6	108.3(8)
L1N6-Co2-L2N1	92.6(5)	Co3-L2O1-L2N6	109.0(8)
L1N6-Co2-L2N6	90.0(5)	Co3-L3O1-L3N6	108.6(7)
L1N6-Co2-L3N1	171.1(5)	Co3-L4O1-L4N6	107.9(8)
L1N6-Co2-L3N6	90.2(5)	Co3-L5O1-L5N6	109.5(7)
L2N1-Co2-L2N6	81.4(5)	Co3-L6O1-L6N6	109.1(7)
L2N1-Co2-L3N1	96.4(5)	Co1-L4N6-L4O1	122.2(9)
Co1-L5N6-L5O1	122.1(8)	L4N6-L4C4-L4C5	122(1)
Co1-L6N6-L6O1	122.0(9)	L5N6-L5C4-L5C5	121(1)
Co2-L1N6-L1O1	121.9(9)	L6N6-L6C4-L6C5	122(1)
Co2-L2N6-L2O1	122.2(8)	L1C2-L1C4-L1C5	127(2)
Co2-L3N6-L3O1	121(1)	L2C2-L2C4-L2C5	124(1)
Co1-L4N6-L4C4	117(1)	L3C2-L3C4-L3C5	124(1)
Co1-L5N6-L5C4	117.2(9)	L4C2-L4C4-L4C5	125(1)
Co1-L6N6-L6C4	118(1)	L5C2-L5C4-L5C5	127(1)
Co2-L1N6-L1C4	118(1)	L6C2-L6C4-L6C5	128(2)
Co2-L2N6-L2C4	117(1)	L1C3-L1C2-L1C4	119(1)
Co2-L3N6-L3C4	116.6(9)	L2C3-L2C2-L2C4	121(1)
L1O1-L1N6-L1C4	120(1)	L3C3-L3C2-L3C4	118(1)
L2O1-L2N6-L2C4	120(1)	L4C3-L4C2-L4C4	121(1)
L3O1-L3N6-L3C4	123(1)	L5C3-L5C2-L5C4	118(1)
L4O1-L4N6-L4C4	121(1)	L6C3-L6C2-L6C4	117(2)
L5O1-L5N6-L5C4	121(1)	L1N1-L1C2-L1C4	117(1)
L6O1-L6N6-L6C4	120(1)	L2N1-L2C2-L2C4	116(1)
L1N6-L1C4-L1C2	111(1)	L3N1-L3C2-L3C4	116(1)

Table 6. (Continued)

Atoms	Degrees	Atoms	Degrees
L2N6-L2C4-L2C2	113 (1)	L4N1-L4C2-L4C4	116 (1)
L3N6-L3C4-L3C2	114 (1)	L5N1-L5C2-L5C4	117 (1)
L4N6-L4C4-L4C2	113 (1)	L6N1-L6C2-L6C4	118 (2)
L5N6-L5C4-L5C2	112 (1)	L1N1-L1C2-L1C3	124 (2)
L6N6-L6C4-L6C2	111 (1)	L2N1-L2C2-L2C3	123 (1)
L1N6-L1C4-L1C5	122 (2)	L3N1-L3C2-L3C3	126 (1)
L2N6-L2C4-L2C5	123 (1)	L4N1-L4C2-L4C3	123 (1)
L3N6-L3C4-L3C5	122 (1)	L5N1-L5C2-L5C3	125 (1)
L6N1-L6C2-L6C3	124 (1)		
Co1-L4N1-L4C2	112.2 (9)		
Co1-L5N1-L5C2	112 (1)		
Co1-L6N1-L6C2	112 (1)		
Co2-L1N1-L1C2	113 (1)		
Co2-L2N1-L2C2	112.4 (9)		
Co2-L3N1-L3C2	113.3 (9)		

distances indicates that the central cobalt can be assigned as cobalt(II).

Thus, two of the three cobalts are oxidized in the absence of air, and presumably some of the ligand is reduced. The same results are obtained in air. Apparently, the field provided by six nitrogens is sufficient to allow the oxidation and reduction to occur, while that provided by six oxygens is not. Only part of the cobalt is oxidized, because there is not enough ligand present to coordinate all the metal.

It is interesting to compare and contrast this structure and that of the previously discussed complex of 2-aminoethanol (see Figure 2). Both consist of two terminal cobalt(III) ions and a central cobalt(II) arranged linearly. Although coordination of the terminal cobalt ions is octahedral in both complexes, coordination at the central cobalt ion differs. Coordination of the central cobalt(II) in the 2-aminoethanol complex is trigonal prismatic and there is two-fold site symmetry (The two tris chelates are of the same optical configuration). This contrasts with the octahedral coordination of the central cobalt(II) in the Dma complex and the absence of symmetry (The approach to a threefold symmetry can be seen in Figure 7).

Another interesting feature is that the 2-aminoethanol complex is formed by oxidation of cobalt(II) in air, while the Dma complex is formed in air or in the absence of

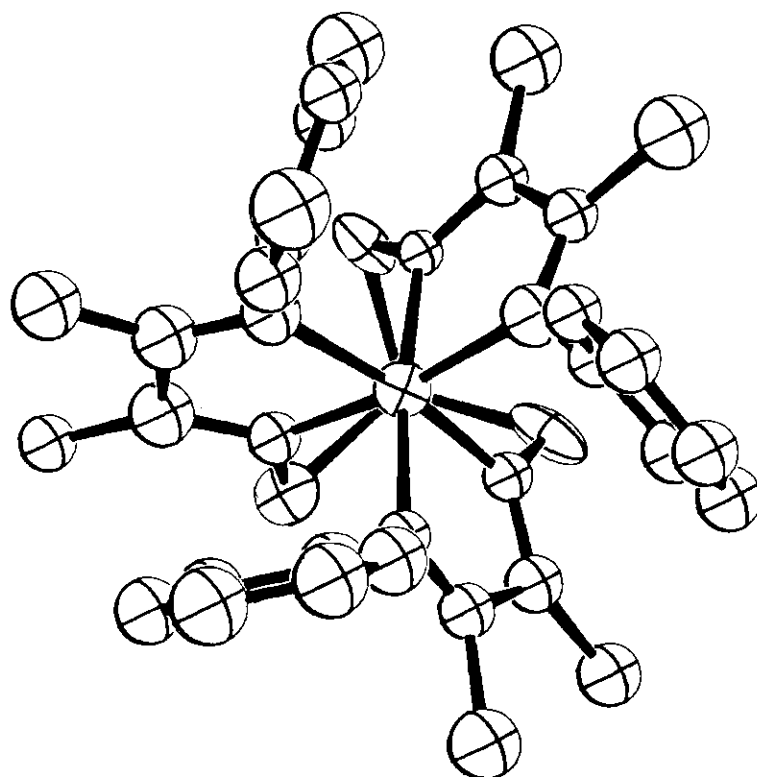


Figure 7. A View of $[\text{Co}_3(\text{Dma})_6](\text{ClO}_4)_2$ Along
the Co(III) - Co(II) Axis (One Co
(III) and Associated Ligands Omitted)

air. The difference lies presumably in the nature of the ligands. As discussed earlier, the field provided by six nitrogens in the Dma complex is apparently sufficient to permit oxidation in the absence of air. However, in the 2-aminoethanol complex, each of the oxidized cobalts is surrounded by three nitrogens and three oxygens. Also, the 2-aminoethanol is less easily reduced than the Dma and this diminishes its ability to serve as an oxidizing agent.

Comparison of the refined structure with measured density, analyses, and residual electron density that could not be refined indicates that something else is present in the crystalline compound. Difficulties involving inconsistent weight loss and cracking of the crystals make a definite interpretation impossible. However, a reasonable explanation would be the presence of disordered solvent and/or water molecules in the crystal. If sufficiently disordered, such molecules would not show up in a difference Fourier calculation.

It should be pointed out that there is not a marked difference between the %C, H, and N for the formula proposed by Uhlig and Dinjus and the values for the actual structure. Their formulation is not unreasonable in the absence of a structure determination.

The magnetic moment per gram atom of cobalt can be recalculated in terms of the new formulation, assuming the cobalt(III) ions are diamagnetic. Although Uhlig and Dinjus

report two different compounds, $[\text{Co}(\text{Dma})(\text{Cma-H})\text{B}]\text{ClO}_4$ where $\text{B} = \text{C}_5\text{H}_5\text{N}$ or $\text{C}_6\text{H}_5\text{NH}_2$, the same compound, $[\text{Co}_3(\text{Dma})_6](\text{ClO}_4)_2$, was obtained using either procedure; crystals from both preparations gave the same unit cell parameters. The recalculated room temperature magnetic moment reported for the aniline complex, 5.17 B.M., is in the normal range for octahedral cobalt(II). However, the value for the pyridine complex, 5.95 B.M., is not in the normal range and can not be explained. No temperature dependence is exhibited since only a single paramagnetic center is present in each formula unit.

CHAPTER IV

CONCLUSION

In reviewing the mixed-valence polynuclear cobalt complexes that have been reported, it can be seen that they fall into two categories; those that exhibit temperature-dependent magnetic moments and those that exhibit temperature independent magnetic properties. In all cases a direct assignment of charge at the cobalt ions has been possible on the basis of bond distances and no delocalization of charge has been evident. $[\text{Co}_3(\text{Dma})_6](\text{ClO}_4)_2$ is consistent with the above and represents another example of a polynuclear cobalt complex with a single paramagnetic center.

Other polynuclear cobalt complexes could probably be prepared using similar ligands and oxidation of the central cobalt would be interesting. Also, replacement of the central cobalt by other metal ions could be attempted.

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